

2. Electrochemical Energy Storage

Improving the batteries for electric drive vehicles, including hybrid electric (HEV) and plug-in electric (PEV) cars, 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 U.S. Department of Energy (DOE) Vehicle Technologies Office (VTO) 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 DOE 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 electrochemistries 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 DOE has conducted in batteries and energy storage. Research supported by VTO 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; and
- Halve the weight of an electric vehicle battery;

Achieving these goals would result in:

- Lowering battery cost from \$500/kwh to \$125/kwh; and
- Increasing energy and power densities 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

DOE received feedback on the overall technical subprogram areas presented during the 2015 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 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: Peter Faguy (U.S. Department of Energy) – es000

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

Reviewer 1:

The reviewer said yes, and that the strategy was covered very well from an automotive original equipment manufacturer (OEM) perspective.

Reviewer 2:

The reviewer remarked that the overview was necessarily brief. The presentation culled out some highlights of what was accomplished and mentioned the goals. The reviewer suggested that more information on why certain areas are being included and excluded would have been helpful. The reviewer believed that successful implementation of electric vehicles is being held up by the difficult material challenges faced. The reviewer believed that a lot of the manufacturing, cost modeling, and even the pack control systems can come along later. Consequently, the 22% of the funding pie for exploratory materials research seems far too low, but the reviewer believed that materials research makes up a large portion of the DOE Funding Opportunity Announcements (38%). If that is indeed the case, then the reviewer approves of the funding split, otherwise the reviewer suggests boosting the materials portion of the pie.

Reviewer 3:

The reviewer found that a general ongoing strategy can be deduced from the projects underway, the projects completed, and future plans. However, there was no overall strategy described that illustrates any particular direction for the future.

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

Reviewer 1:

The reviewer pointed out that the automotive industry has a long lead time for implementation of new technology. The time frames provided establish time periods that appear to fit the near-, mid-, and mid-long term research development schedules.

Reviewer 2:

The reviewer was impressed with the wide range of the programs being funded within the near- and mid-term implementation timeline (5-15 years). The reviewer agreed with leaving much longer-term prospects for vehicle applications, such as magnesium and lithium-air batteries, to other programs, such as Advanced Research Projects Agency - Energy (ARPA-E) and Joint Center for Energy Storage Research (JCESR) that can better accommodate the much higher risks associated with such systems. The program is focused on an array of anodes and cathodes, but costing and energy/power requirements are being used to direct the work so that it is not wasted on systems/materials that have no hope of meeting the targets. The reviewer believed that in almost all areas, if the projects were to be successful, they would be very impactful (i.e., “if you had, you would indeed want it”). Thus, the reviewer thinks that the program managers have used a very disciplined approach to select projects with varying degrees of risk that are yet generally aligned with the program goals. The reviewer pointed out that some of the method development in this program is outstanding and should provide valuable tools to really understand what is going on in these systems for many years to come.

Reviewer 3:

The reviewer suggested greater focus on near-term research & development (R&D) and manufacturing issues, and more advanced fundamental science, rather than on mid-term R&D can better position the United States in this industry.

Question 3: Were important issues and challenges identified?

Reviewer 1:

The reviewer said yes, and explained that frankly, everyone knows the challenges and issues.

Reviewer 2:

The reviewer found that most of the key high-voltage battery issues were identified, such as the need for the key cell components (cathode and electrolyte in particular) to have high voltage capability; the need for improvement in the anode to obtain higher energy density by using silicon; and improvement in manufacturing/processes to reduce overall cell/system cost.

Reviewer 3:

The reviewer said that issues and challenges were identified at a high level.

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

Reviewer 1:

The reviewer said yes, the plans were identified to address the issues and challenges. This was done by offering various funding opportunities; identifying multiple paths that offer potential solutions; and, finally providing the appropriate funding method to help respondents prove out their proposed solution.

Reviewer 2:

The reviewer said that plans were identified at a high level.

Reviewer 3:

The reviewer thinks that the goals are clear and the presentation touches on some of the highlights, but there was little in there on details of the overall plan. The reviewer was happy with the portfolio of projects being undertaken, and presumably this is a reflection of DOE's planning in this area, but the plans were not explicitly discussed in any depth, at least not that the reviewer can recall. The reviewer presumed plans are laid out in detail in some of the extremely large documents on VTO's website, but there really was no time to get into this during the time allotted for the presentation.

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

Reviewer 1:

The reviewer found that the progress while not clearly benchmarked against the previous year were sufficiently identified. The reviewer pointed out that the addition of the U.S. Advanced Battery Consortium (USABC) programs was added, new testing efforts were added, and the computer-aided engineering of batteries (CAEBAT) efforts were added.

Reviewer 2:

The reviewer said yes, but at a very general and very high level. The reviewer thought the level was too high and too general.

Reviewer 3:

The reviewer said not really, although progress versus the goals was fairly clear. In terms of progress since last year, the reviewer said that cost estimates of packs are much more developed, as is the modeling of battery pack performance under CAEBAT. There was also some very interesting method development going on. The reviewer pointed out that some of the advances in getting silicon to cycle look promising, but translating this into commercial cells seems to be a major hurdle that remains elusive. The reviewer did not believe that the cathode work or electrolyte work showed major advances, although the reviewer thought some of the projects look very promising so maybe next year they will bear fruit.

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 noted that the projects that have been selected are addressing the issues that were identified earlier.

Reviewer 2:

The reviewer said yes.

Reviewer 3:

The reviewer said yes, and elaborated that in almost every case the reviewer understood the point of why the project was funded.

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

Reviewer 1:

The reviewer emphatically said yes.

Reviewer 2:

The reviewer found that the focus could be much greater and could be significantly improved, but it is effective in addressing VTO's needs

Reviewer 3:

The reviewer believed that the projects are in general worthwhile and targeted at the main problems. The reviewer cautioned that despite the following criticisms, overall the reviewer thought the program team is doing a very good job in managing the project portfolio.

Notwithstanding the above, the reviewer believed that some of the costing work is overkill. The reviewer noted that the models of plant costs seemed acceptable, but some of the items DOE was looking at were pretty unimportant (cutting maybe \$25 from a car battery pack). The reviewer suggested that perhaps the outcome is unknown until models are run, but the reviewer thinks this could really be left to industry, which obsesses about running efficient plants 24/7. The reviewer said that most of the costs still seem to be in raw materials, and asked if energy costs are really that important.

The reviewer cited modeling work as the biggest problem. The reviewer noted that the program includes a wide array of modeling, all the way from ab initio modeling of atoms to thermal/electrical modeling of complete battery packs. Taken individually, the reviewer had no issue with the various projects being taken. However, the reviewer believed that the efforts remain far too uncoordinated. Basic problems the reviewer cited are that: there does not seem to be a master plan of the desired future state of the modeling activities; modelers seem to be doing what they can or want to do, not what needs to be done; and communication among the modelers seems poor, especially among different programs within the DOE. The reviewer applauded the CAEBAT effort to rein in these disparate modeling initiatives, this is really making the best of a bad situation. The reviewer believes that fundamentally, the issues are mainly a result of the proposal-driven funding mechanism used by DOE (and many other government agencies). While this mechanism has of course some merits, the reviewer believed it has led to many uncoordinated and in some cases competing efforts.

Ideally, the reviewer would like to see a comprehensive evaluation and outlining of what exactly the program actually needs in the various modeling areas and then assignments made to the groups best positioned to address those needs. The reviewer does not believe that the request for proposals really do this in any truly coordinated way. The reviewer appreciates that such an approach may not be viable for a government run program, but the modeling efforts badly need more oversight and control. The reviewer suggested maybe

having a modeling czar selected from one of the experienced modelers in the middle of the micro-meso-macro scale of models to help create such a plan, and suggested maybe Dennis Dees.

If, as is likely, such an approach cannot be taken, the reviewer suggested continuing to support the CAEBAT program that at least tries to make sure the programs standardize on the language, etc. Regardless of the above strategy, the reviewer believed that there should be much more frequent communications among the modelers at all levels and across all programs. While there is of course a big difference between the type of modeling at the ab initio versus pack level, the reviewer believed that more frequent working meetings to share what modelers are doing would be very beneficial. The reviewer pointed out that some of the modelers do not seem to know what others are doing until they come to the Annual Merit Review (AMR).

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:

The reviewer identified as a key weakness the lack of responders to the proposals that have a strong chance of meeting the proposal requirements. The reviewer is unsure if this is because of the requirements in the Funding Opportunity Announcements (FOAs)/request for proposal information (RFPIs) or something else. The reviewer said that the strengths are the variety of opportunities that are offered and the quick response when new technology needs are identified. This variety in funding and quick response is evident in the USABC project/program as other opportunities were opened to allow for additional responses. The reviewer detailed that this was done by developing new RFPIs in concert with DOE, without much overlapping with DOE's existing FOAs.

Reviewer 2:

The reviewer pointed out that battery manufacturing initiatives, Battery Materials Research, and USABC stand out as the most useful aspects.

Reviewer 3:

The reviewer thinks the strengths of many of the programs are their originality and focus on the main issues at hand. The reviewer thought that the following projects were excellent. Mike Thackeray's talk (es049) was very promising, and the reviewer believed that while the lithium-manganese rich (LMR) material might never be able to deliver its original potential capacity while retaining the cycle life needed for vehicle applications, taking a small cut in capacity to attain the stability needed would nevertheless be a huge step forward.

The reviewer supported Stanley Whittingham's work on alternate anodes that are less reactive than lithiated silicon. The reviewer remains very concerned that after more than a decade of extensive work, silicon (Si) anodes are only being used in very small amounts in consumer applications (LG and Samsung) where cycle life demands are far less rigorous. The reviewer pointed out that despite all the work showing good cycle life of Si anodes, getting stable performance in a full cell still seems to be very challenging. The reviewer thought that Clare Grey's nuclear magnetic resonance (NMR) work and method development seemed truly groundbreaking. The reviewer cited various projects to extend in situ diagnostic methods to run in operando. The reviewer thought that Andrew Jansens's poster (es030) on the Cell Analysis, Modeling, and Prototyping (CAMP) lab at Argonne National Laboratory (ANL) showed that the team has been extremely productive and are providing a valuable service to the community. More importantly, the reviewer thought that the team appears to be involved in planning the work. This is a crucial involvement to both ensure relevance of the work and good data interpretation.

The reviewer was impressed by Dean Wheeler and Brian Mazzeo's work (es220). The reviewer found that the method he and his partner have devised to map the electronic conductivity of an electrode is very important to the industry. Uneven current distributions in cells from non-uniform electrodes can reduce cycle life and/or lead to lithium plating. The reviewer provided as an example, at the spring 2015 ECS meeting a few weeks ago, Tobias Bach showed how the pressure from just the tab of a cell can lead to non-uniform discharge currents that then greatly reduce cycle life. Stephen Harris and others have also highlighted the importance of

having uniform electrodes. Developing their method to also map ionic conductivity would also be an invaluable extension of this method. The reviewer pointed out the ab initio modeling work at Lawrence Berkeley National Laboratory (LBNL) and Massachusetts Institute of Technology (MIT). The reviewer thought that what was great was the project team can explain their results and especially provide insight that cannot often be achieved from experiments – not just results. The reviewer thought that Kevin Gallagher’s paper presented by Dennis Dees also provided valuable insight.

The reviewer pointed out various initiatives looking at lower cost and/or radically different ways to make electrodes. About new electrodes, the reviewer said that this is a difficult area where little has really changed over the last 20 years or so, but the reviewer credited VTO for putting together a surprisingly good selection of projects that are really very innovative. The reviewer said that the use of ionic liquids as an electrolyte for lithium-oxygen by Vincent Giordani (LIOX, es233) was interesting, as long as the energy losses to keep the pack warm would be acceptable.

The reviewer thought there were somewhat weak areas. According to the reviewer, the car battery market will not really take off until battery costs come down. Because raw materials costs still dominate, this means less expensive raw materials and this in turn is likely to make it uneconomic to recycle these batteries for their components. However, undesirable it would be from an environmental or resource issue, it may well end up being cheaper to just dig up more stuff from the ground than to recycle. The reviewer suggested that DOE should be focused on developing policies to address this, although maybe this is not VTO’s role. The reviewer believed that most Western countries will simply mandate recycling and thus the costs for this will actually have to be added in to the production in costs for the battery because the reviewer does not believe recycling these batteries may ever be profitable. Another option that the reviewer presumes will not come to pass even in the United States, is not requiring recycling, but leave the landfilling open as an option, but the reviewer noted that again this cost should be including in the battery costs.

The reviewer identified modeling of plant costs, and elaborated that models seemed acceptable, but some of the items examined were pretty unimportant, such as cutting maybe \$25 from a car battery pack. The reviewer suggested that perhaps the outcome is unknown until models are run, but the reviewer thinks this could really be left to industry, which obsesses about running efficient plants 24 hours a day, 7 days a week. Most of the costs still seem to be in raw materials. The reviewer said that the work at Argonne to find a new organic solvent (es066) did not seem to be coming up with anything new. The reviewer pointed out es215 and suggested that, being new to the field, this principal investigator (PI) would benefit from a much closer working relationship with existing partners at Berkeley.

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

Reviewer 1:

The reviewer said yes, these projects do represent novel ways. The reviewer said that the goals in the FOAs and the RFPIs are sufficiently aggressive to drive the need to develop novel/innovative solutions to meet the target.

Reviewer 2:

The reviewer said that some projects do.

Reviewer 3:

The reviewer would generally characterize the approaches as quite innovation and a credit to DOE's program. The reviewer believed that not enough attention is given to some of the drawbacks of the nano-approaches so prevalent in terms of poor packing; high surface area and the reactivity associated with that; energy and power on a volume as well as weight basis; electrolyte needed to wet all the surfaces; and costs

Question 10: Has the program area engaged appropriate partners?

Reviewer 1:

The reviewer said that the program has an excellent group of partners. The reviewer cited automotive original equipment manufacturers (OEMs), battery manufacturers, and battery component suppliers are included and address the near- and mid-term needs; while universities, national laboratories, and research companies cover in particular the long-term research concerns.

Reviewer 2:

The reviewer said that as restricted by DOE's governmental restrictions, yes. However, according to the reviewer the entire program could much better position the United States and U.S. industries if greater allowance and initiative for international partnership and collaboration was enacted.

Reviewer 3:

The reviewer said yes, and elaborated that VTO has a wide range of industrial partners in both materials, processing and pack assembly. The reviewer wished that LG and Samsung or some Japanese companies were more involved because they can bring a lot of realism to the party, but the reviewer understands that this is not very attractive in terms of developing a U.S.-based supply chain. The reviewer noted that these companies may not be willing to contribute much due to the competitive nature of their business. The reviewer said that the national laboratories and universities are all pulling their weight and contributing to the program.

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

Reviewer 1:

The reviewer said yes, the program is collaborating very well with all of the partners.

Reviewer 2:

The reviewer was amazed at the sheer number of collaborators listed on some posters and talks. The reviewer suspected that this is in part due to the prominence this is given in the reviewing form. The reviewer noted that collaboration requires some investment in time and money, so the reviewer could see that in some cases maybe project teams actually have too many. The reviewer does not believe that collaboration should be an end of itself.

The reviewer pointed out that the big question is how effective are the collaborations and it is very hard to tell that from the presentations. A promising indicator was that several PIs told this reviewer the project teams have regular meetings with the stakeholders and other researchers to discuss progress, which the reviewer thinks is great, especially if meetings can be kept informal and focused on technical not managerial aspects. Others conveyed to this reviewer that project teams received valuable guidance from their partners.

Based on this, the reviewer believes that the collaboration is actually working out very well. The reviewer noted es215, and that with this PI being new to the field, this PI would benefit from a much closer working relationship with existing partners at Berkeley. The reviewer expressed concern that this PI seemed far too unaware of what the field is doing and trying to do.

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

Reviewer 1:

The reviewer said that there are no obvious gaps in the key technology areas.

Reviewer 2:

The reviewer understands the Bollere Li-vanadium oxide battery systems are being used in France, and asked if DOE is talking with these folks. Stability of a protected lithium anode to physical abuse and consequences of the film rupture during such events. The reviewer would like to know how well these films are likely to stand up to a crash scenario.

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

Reviewer 1:

The reviewer said that there is no clear lack of depth in the work for any of the identified topics.

Reviewer 2:

The reviewer cited electrolytes, separators, and advanced anodes with more and international partners

Reviewer 3:

The reviewer would like to see a better understanding of why exactly the advanced silicon anodes are not making into commercial cells, especially those for consumer devices where 300-500 cycles is often adequate. The reviewer would like to know if the barrier is the physical expansion and/or chemical side reactions. The reviewer pointed out that assumptions made of lithium metal cells depend very much on the efficiency used and the amount of excess lithium that is then required. The reviewer asked how this is factored into energy density/specific energy estimates. The reviewer recommended that Vince Battaglia (es232) should run a test of cell reproducibility either by making and testing a large batch of control cells (say 10) or better by including 2 control cells in each of the experiments and over time building up a database. The reviewer believed this would capture run-to-run as well as within-a-run variability. The reviewer stipulated that maybe the PI already has this, but the PI said not.

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

Reviewer 1:

The reviewer said yes, and cited relationship and partnering of consumer electronics manufacturers and cell manufacturers with automotive and automotive-related participants.

Reviewer 2:

The reviewer said that fast charging has received some attention; however, one area that may need to be addressed is the quick removal of stranded energy from batteries that may have been involved in an accident. This area is in particular to address safety concerns, but may drive technology improvements in many areas or/and drive design commonality in some areas. The reviewer suggested that the effect that fast charging has on battery safety and battery life should be considered for future work.

Reviewer 3:

The reviewer suggested creating an overall master plan for the various modeling initiatives

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

Reviewer 1:

The reviewer cannot think of any new ways to approach these barriers.

Reviewer 2:

The reviewer suggested increasing relative funding to allow for continued funding of national laboratories at similar levels while increasing relative funding to industrial partners in the United States and internationally.

Reviewer 3:

The reviewer thought Wildcat Technologies' high throughput methodology is tailor made to looking at electrolyte and other additives. The reviewer strongly encouraged that this organization be tasked to take a look at this. In the reviewer's view, this entity has a very good track record.

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

Reviewer 1:

The reviewer cannot think of any at this time.

Reviewer 2:

The reviewer noted that there seems to be some issues with the basic understanding of ANL's LMR cathode between Berkeley and other labs regarding the presence of microdomains of LiMn_2O_3 . The reviewer noted that while disagreements are fine, the reviewer believed that the groups are talking past each other via publications and not directly with each other. The reviewer believed the program managers should try and force the issue to see whether a consensus can be reached, i.e., identify who's right. The reviewer acknowledged that sometimes there is not enough information to take this approach, but the reviewer believed that with all the studies being done on this material, there should be enough information to come to a resolution.

The reviewer expressed concern that Nancy Dudney's work (es182) seems to have progressed a bit slowly. The reviewer thinks this is important and that the PI may need an extension to complete the work properly. The reviewer fears there is still far too much to do before the funding runs out. The reviewer said that those developing new methods seem to be rushed to apply them to lots of materials right away, presumably to show relevance and highlight the importance of the work. The reviewer fears the project teams are rushing into the application field too quickly, before the teams have really done a thorough job of validating the method. The reviewer was happy to see that Clare Grey's group took a time-out to look at their methods in such detail.

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 |
|---|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Novel Cathode Materials and Processing Methods | Thackeray, Michael (ANL) | 2-22 | 3.50 | 3.67 | 3.83 | 3.67 | 3.65 |
| High-Capacity, High-Voltage Cathode Materials for Lithium-Ion Batteries | Manthiram, Arumugam (U of Texas at Austin) | 2-25 | 3.00 | 3.00 | 2.67 | 2.83 | 2.94 |
| Design of High-Performance, High-Energy Cathode Materials | Doeff, Marca (LBNL) | 2-28 | 3.17 | 3.50 | 3.67 | 3.17 | 3.40 |
| First Principles Calculations of Existing and Novel Electrode Materials | Ceder, Gerbrand (Massachusetts Institute of Technology) | 2-31 | 3.83 | 3.67 | 3.67 | 3.50 | 3.69 |
| First Principles Calculations and NMR Spectroscopy of Electrode Materials | Grey, Clare (U. of Cambridge) | 2-34 | 3.50 | 3.33 | 3.50 | 3.17 | 3.38 |
| Development of High-Energy Cathode Materials | Zhang, Jason (PNNL) | 2-37 | 3.00 | 3.17 | 3.50 | 2.67 | 3.10 |
| Advanced In-Situ Diagnostic Techniques for Battery Materials | Yang, Xiao-Qing (BNL) | 2-41 | 3.00 | 3.17 | 3.33 | 3.00 | 3.13 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|--|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Development of Novel Electrolytes and Catalysts for Lithium-Air Batteries | Amine, Khalil (ANL) | 2-44 | 3.67 | 3.50 | 3.67 | 3.67 | 3.58 |
| Design and Scalable Assembly of High-Density Low-Tortuosity Electrodes | Chiang, Yet-Ming (Massachusetts Institute of Technology) | 2-47 | 3.13 | 3.38 | 3.13 | 3.25 | 3.27 |
| Interfacial Processes in EES Systems Advanced Diagnostics | Kostecki, Robert (LBNL) | 2-50 | 3.67 | 3.83 | 3.50 | 3.67 | 3.73 |
| Predicting and Understanding Novel Electrode Materials From First Principles | Persson, Kristin (LBNL) | 2-53 | 3.67 | 3.67 | 3.67 | 3.50 | 3.65 |
| Studies on High Capacity Cathodes for Advanced Lithium-Ion Systems | Nanda, Jagjit (ORNL) | 2-56 | 3.00 | 3.33 | 3.67 | 3.00 | 3.25 |
| PHEV and EV Battery Performance and Cost Assessment | Gallagher, Kevin (ANL) | 2-59 | 3.50 | 3.70 | 3.20 | 3.40 | 3.55 |
| Open Architecture Software for CAEBAT | Turner, John (ORNL) | 2-62 | 3.00 | 3.00 | 2.83 | 2.83 | 2.96 |
| Composite Electrolytes to Stabilize Metallic Lithium Anodes | Dudney, Nancy (ORNL) | 2-65 | 2.75 | 2.75 | 3.00 | 2.75 | 2.78 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|---|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| In-Situ Solvothermal Synthesis of Novel High Capacity Cathodes | Wang, Feng (BNL) | 2-68 | 3.00 | 3.00 | 3.67 | 2.83 | 3.06 |
| Lithium Bearing Mixed Polyanion Glasses as Cathode Materials | Kercher, Andrew (ORNL) | 2-71 | 3.00 | 2.83 | 3.17 | 2.83 | 2.92 |
| Significant Enhancement of Computational Efficiency in Nonlinear Multiscale Battery Model for Computer Aided Engineering † | Kim, Gi-Heon (NREL) | 2-74 | 3.67 | 3.67 | 3.17 | 3.17 | 3.54 |
| Mechanistic Modeling Framework for Predicting Extreme Battery Response: Coupled Hierarchical Models for Thermal, Mechanical, Electrical and (Electro)Chemical Processes † | Moffat, Harry (SNL) | 2-77 | 3.83 | 3.33 | 3.50 | 3.17 | 3.46 |
| Coupling Mechanical with Electrochemical-Thermal Models Batteries under Abuse † | Pesaran, Ahmad (NREL) | 2-80 | 3.83 | 3.33 | 3.33 | 3.50 | 3.48 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Efficient Safety and Degradation Modeling of Automotive Lithium-Ion Cells and Pack † | Shaffer, Christian (EC-Power) | 2-83 | 3.00 | 3.00 | 3.00 | 2.67 | 2.96 |
| Electrochemical Performance Testing † | Bloom, Ira (ANL) | 2-86 | 3.50 | 3.50 | 3.75 | 3.50 | 3.53 |
| INL Electrochemical Performance Testing † | Christophersen, Jon (INL) | 2-88 | 3.75 | 3.75 | 4.00 | 4.00 | 3.81 |
| Battery Safety Testing † | Orendorff, Christopher (SNL) | 2-90 | 4.00 | 3.75 | 4.00 | 4.00 | 3.88 |
| Battery Thermal Characterization † | Keyser, Matthew (NREL) | 2-92 | 3.25 | 3.50 | 3.25 | 3.50 | 3.41 |
| New High-Energy Electrochemical Couple for Automotive Applications † | Amine, Khalil (ANL) | 2-94 | 3.38 | 3.50 | 3.38 | 3.50 | 3.45 |
| High-Energy High-Power Battery Exceeding PHEV-40 Requirements † | Rempel, Jane (TIAX) | 2-98 | 3.00 | 2.88 | 2.75 | 2.50 | 2.84 |
| Advanced High-Energy Lithium-Ion Cell for PHEV and EV Applications † | Singh, Jagat (3M) | 2-102 | 3.13 | 3.13 | 3.38 | 3.13 | 3.16 |
| High-Energy Lithium Batteries for PHEV Applications † | Venkatachala, Subramanian (Envia) | 2-105 | 3.38 | 3.38 | 3.38 | 3.25 | 3.36 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| High-Energy, Long Cycle Life Lithium-Ion Batteries for PHEV Applications † | Wang, Donghai (Penn State) | 2-108 | 3.00 | 3.00 | 3.00 | 3.00 | 3.00 |
| High Energy Density Lithium-Ion Cells for EV's Based on Novel, High Voltage Cathode Material Systems † | Kepler, Keith (Farasis) | 2-112 | 3.50 | 3.50 | 3.50 | 3.38 | 3.48 |
| First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anodes | Balbuena, Perla (Texas A&M) | 2-115 | 3.17 | 3.17 | 3.00 | 2.83 | 3.10 |
| Analysis of Film Formation Chemistry on Silicon Anodes by Advanced In Situ and Operando Vibrational Spectroscopy | Somorjai, G. (UC Berkeley) | 2-118 | 3.17 | 3.00 | 2.50 | 3.17 | 3.00 |
| Optimization of Ion Transport in High-Energy Composite Cathodes | Meng, Shirley (UC San Diego) | 2-121 | 3.50 | 3.25 | 3.75 | 3.50 | 3.41 |
| Daikin Advanced Lithium-Ion Battery Technology - High-Voltage Electrolyte | Hendershot, Ron (Daikin America) | 2-125 | 3.50 | 3.67 | 2.67 | 3.33 | 3.46 |
| Fluorinated Electrolyte for 5 V Lithium-Ion Chemistry | Zhang, John (ANL) | 2-128 | 3.33 | 3.00 | 3.00 | 2.83 | 3.06 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|---|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Novel Non-Carbonate Based Electrolytes for Silicon Anodes | Strand, Dee (Wildcat Discovery) | 2-131 | 3.17 | 3.33 | 3.50 | 3.00 | 3.27 |
| Predicting Microstructure and Performance for Optimal Cell Fabrication | Wheeler, Dean (BYU) | 2-134 | 3.38 | 3.25 | 3.25 | 3.13 | 3.27 |
| A Combined Experimental and Modeling Approach for the Design of High Coulombic Efficiency Si Electrodes | Xiao, Xingcheng (GM) | 2-137 | 3.33 | 3.17 | 3.33 | 2.83 | 3.19 |
| Electrode Architecture-Assembly of Battery Materials and Electrodes | Zaghib, Karim (Hydro Quebec) | 2-140 | 3.25 | 3.38 | 3.38 | 3.13 | 3.31 |
| Hierarchical Assembly of Inorganic/Organic Hybrid Si Negative Electrodes | Liu, Gao (LBNL) | 2-143 | 3.88 | 3.75 | 3.75 | 3.38 | 3.73 |
| Simulations and X-ray Spectroscopy of Lithium-Sulfur Chemistry | Balsara, Nitash (LBNL) | 2-146 | 3.25 | 3.00 | 3.13 | 2.88 | 3.06 |
| Design and Synthesis of Advanced High-Energy Cathode Materials | Chen, Guoying (LBNL) | 2-149 | 3.33 | 3.50 | 3.50 | 3.33 | 3.44 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Microscopy Investigation on the Fading Mechanism of Electrode Materials | Wang, Chongmin (PNNL) | 2-152 | 3.88 | 3.88 | 3.88 | 3.50 | 3.83 |
| BatPaC Model Development | Ahmed, Shabbir (ANL) | 2-155 | 3.50 | 3.67 | 3.33 | 3.42 | 3.55 |
| Lithium-Ion Battery Production and Recycling Materials Issues | Gaines, Linda (ANL) | 2-159 | 3.50 | 3.42 | 2.83 | 2.92 | 3.30 |
| Sulfur Cathode for Lithium Sulfur Batteries | Cui, Yi (Stanford University) | 2-163 | 3.25 | 3.25 | 3.13 | 3.13 | 3.22 |
| High Energy Density Lithium Battery | Whittingham, Stanley (Binghamton U.-SUNY) | 2-166 | 3.50 | 3.13 | 3.00 | 3.13 | 3.20 |
| Electrode Fabrication and Performance Benchmarking | Battaglia, Vincent (LBNL) | 2-169 | 3.00 | 3.50 | 3.38 | 3.13 | 3.31 |
| Efficient Rechargeable Li/O ₂ Batteries Utilizing Stable Inorganic Molten Salt Electrolytes | Giordani, Vincent (Liox) | 2-172 | 3.50 | 3.17 | 3.33 | 3.33 | 3.29 |
| Continuum Modeling as a Guide to Developing New Battery Materials | Srinivasan, Venkat (LBNL) | 2-175 | 3.50 | 3.33 | 3.17 | 3.50 | 3.38 |
| Energy Storage Materials Research Using DOE's User Facilities | Thackeray, Michael (ANL) | 2-177 | 3.17 | 3.00 | 3.17 | 2.83 | 3.04 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|---|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Crash Propagation Simulations and Validation † | Santhanagopalan, Shriram (NREL) | 2-180 | 3.25 | 3.50 | 3.25 | 3.25 | 3.38 |
| XG Sciences: Development of Silicon Graphene Composite Anode † | Privette, Robert (XG Sciences) | 2-182 | 3.50 | 3.33 | 3.67 | 3.50 | 3.44 |
| Low-Cost, High-Capacity Lithium-Ion Batteries through Modified Surface and Microstructure † | Zhang, Pu (Navitas Systems) | 2-184 | 3.17 | 2.83 | 2.00 | 3.00 | 2.83 |
| Scale-Up of Low-Cost Encapsulation Technologies for High-Capacity and High-Voltage Electrode Powders † | King, David (Pneumaticoat Technologies) | 2-186 | 3.67 | 3.50 | 2.50 | 3.33 | 3.40 |
| Development of Silicon Graphene Composite Anode † | Mayekar, Samir (Sinode Systems) | 2-188 | 3.50 | 3.33 | 3.50 | 3.17 | 3.38 |
| A Disruptive Concept for a Whole Family of New Battery Systems † | Roumi, Farshid (Parthian Energy) | 2-190 | 2.33 | 1.67 | 1.00 | 2.00 | 1.79 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|--|-------------|----------|---------------------------|----------------|-----------------|------------------|
| Dramatically Improve the Safety Performance of Lithium-Ion Battery Separators and Reduce the Manufacturing Cost using Ultraviolet Curing and High Precision Coating Technologies † | Arnold, John (Miltec UV International) | 2-192 | 2.83 | 2.33 | 2.00 | 1.83 | 2.35 |
| Low-Cost, High-Capacity Non-Intercalation Chemistry Automotive Cells † | Jacobs, Alex (Sila Nanotechnologies) | 2-195 | 3.00 | 3.13 | 2.50 | 2.50 | 2.94 |
| Low-Cost, Structurally Advanced Novel Electrode and Cell Manufacturing † | Tan, Taison (24M Technologies) | 2-198 | 2.17 | 2.17 | 2.00 | 2.33 | 2.17 |
| Advanced Drying Process for Lower Manufacturing Cost of Electrodes † | Ahmad, Iftikhar (Lambda Technologies) | 2-200 | 3.13 | 3.13 | 3.00 | 2.63 | 3.05 |
| EV Battery Development † | Lopez, Herman (Envia Systems) | 2-203 | 3.50 | 3.50 | 3.50 | 3.00 | 3.44 |
| Development of a PHEV Battery † | Busbee, John (Xerion Advanced Battery Corporation) | 2-206 | 2.33 | 2.17 | 2.50 | 2.33 | 2.27 |
| Battery Development † | Alamgir, Mohamed (LG Chem Power) | 2-209 | 3.17 | 2.83 | 2.83 | 3.17 | 2.96 |
| A Commercially Scalable Process for Silicon Anode Prelithiation † | Stefan, Ionel (Amprius) | 2-212 | 3.50 | 2.83 | 3.17 | 3.33 | 3.10 |

| Presentation Title | Principal Investigator and Organization | Page Number | Approach | Technical Accomplishments | Collaborations | Future Research | Weighted Average |
|--|---|-------------|-------------|---------------------------|----------------|-----------------|------------------|
| 12 V SS Battery Development † | Everett, Michael (Maxwell) | 2-215 | 3.17 | 2.67 | 2.83 | 3.00 | 2.85 |
| New High-Energy Electrochemical Couple for Automotive Application † | Yang, Xiao-Qing (BNL) | 2-218 | 3.63 | 3.63 | 3.50 | 3.50 | 3.59 |
| 3M IC3P - Research Focus † | Singh, Jagat (3M) | 2-221 | 3.13 | 3.00 | 2.75 | 2.63 | 2.95 |
| Ion-Exchanged Derived Cathodes (IE-LL_NCM) for High-Energy Density Lithium-Ion Batteries † | Johnson, Christopher (ANL) | 2-224 | 3.50 | 3.13 | 3.00 | 3.00 | 3.19 |
| Envia IC3P - Research Focus † | Kostecki, Robert (LBNL) | 2-227 | 3.38 | 3.50 | 3.38 | 2.88 | 3.38 |
| Prospects and Challenges of Nickel-Rich Layered Oxide Cathodes † | Manthiram, Arumugam (U of Texas at Austin) | 2-230 | 3.50 | 3.25 | 3.00 | 3.13 | 3.27 |
| Materials Development for High Energy High Power Battery Exceeding PHEV-40 Requirements † | Rempel, Jane (TIAX) | 2-233 | 3.00 | 3.00 | 2.63 | 3.00 | 2.95 |
| Overall Average | | | 3.30 | 3.23 | 3.17 | 3.11 | 3.23 |

Note: † denotes poster presentation.

Novel Cathode Materials and Processing Methods: Michael Thackeray (Argonne National Laboratory) - es049

Presenter

Michael Thackeray, Argonne National Laboratory.

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 is good fundamental research to understand the phase transition mechanisms, in the opinion of this reviewer.

Reviewer 2:

Although the concept of tailoring the bulk structure is very sound, and in fact may be the only option, and although early results show some promise with regard to reduction in voltage fade, jury is still out, the reviewer said, on the overall efficacy of this stabilization approach. There is currently no data, the reviewer continued, on oxygen evolution, manganese (Mn) dissolution and corresponding life data, all of which are significant drawbacks of the layered lithium (LL) materials. Thus, the reviewer concluded that it is too early to comment on how effective this approach will be.

Reviewer 3:

The objective here, the reviewer said, is to develop structurally integrated cathode structures, layered-layered-spinel, to overcome the issues inherent in layered-layered composite cathodes, especially voltage fade. The approach is to embed a spinel component of six to 15% into the layered-layered structure, and further stabilize the electrode with a suitable surface coating, the reviewer went on, adding that the latter approach is not as novel. Considering the problems encountered with layered-layered composite electrodes, this approach may provide a viable pathway, in the reviewer’s opinion. However, the reviewer noted, there is considerable reduction both in the cell capacity (approximately 200 mAh/g) and energy (low discharge voltage), so these materials may not compete well with simple, surface-treated, nickel (Ni)-rich layered cathodes operating at these voltages, especially with comparable electrode loadings. The expectation is that thermal stability will be better with the current materials, according to the reviewer, but a proper comparison is required to better understand the benefits here. On the other hand, the reviewer noted, these studies provide an excellent platform to understand Mn-based composite cathodes.

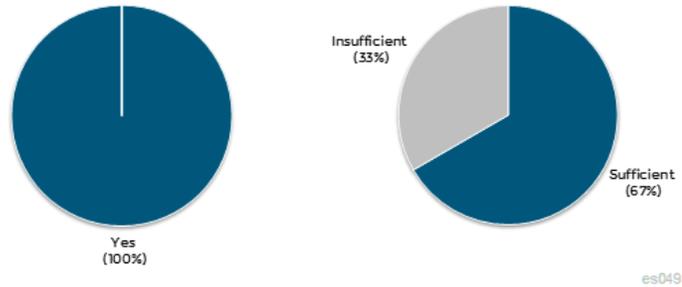
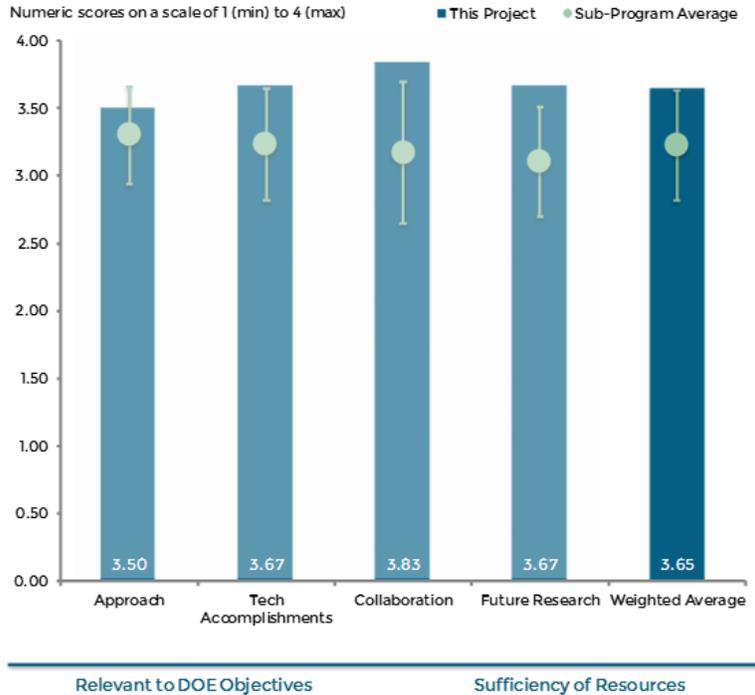


Figure 2-1 Novel Cathode Materials and Processing Methods: Michael Thackeray (Argonne National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

Early results are excellent compared to previous data, the reviewer said, but many key data are needed to make an overall judgement are still missing, so excitement would be premature. Information the reviewer regards as missing includes high-temperature performance, especially life, power over state of charge (SOC) and Mn dissolution, among others. Missing also, according to the reviewer, are data on the surface properties of the TM of these new materials. Finally, the reviewer wondered if there is any difference in the oxidation state of the surface TM of this material versus the baseline materials.

Reviewer 2:

Excellent progress has been made in designing the layered-layered cathodes with embedded spinel component, the reviewer observed, and with such an embedded spinel component (of 6%), and with low cobalt (Co) content, good cyclic stability was demonstrated without the onset of voltage fade, albeit with a lower charge voltage. It appeared to the reviewer to be more prudent to target lower capacities of 220 mAh/g with these materials, as opposed to capacities above 250 mAh/g anticipated for the lithium-manganese rich (LMR)-layered-layered-composite (LLC) material. The designed composite structures with domains of layered and spinel phases were confirmed, the reviewer noted, through X-ray diffraction (XRD) and high-resolution transmission electron microscopy (HRTEM). The reviewer also noted a few good publications that had emerged from this project. The reviewer offered several comments, however. The reviewer asked why the magnesium (Mg)-doped, layered-layered-spinel (LLS), which showed higher capacity/rate capability, was not being pursued. Noting evidence for the local domains of spinel and layered phases, the reviewer asked if it would be possible to verify whether the spinel content (in the bulk) is close to the targeted 6%. The electrode loading should be mentioned/tracked here, the reviewer stated, as the performance is significantly reduced at high loadings with LLC cathodes. Finally, the reviewer questioned why the coating studies focused as much on lithium cobalt oxide (LiCoO₂) cathodes, rather than these cathodes directly.

Reviewer 3:

The reviewer said understand layered spinel structural cathode materials.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Good collaboration, the reviewer said.

Reviewer 2:

There are good collaborations with several researchers from the Argonne National Laboratory and also with external researchers in understanding these materials at the fundamental level, the reviewer opined. However, the reviewer continued, it is probably more appropriate and timely to collaborate closely with the industry, especially the licensees (BASF, Toda, LG and Envia) to establish the merit/relevance of these materials compared to NCA (nickel cobalt aluminum oxide)-based cathodes or LMR-LLC cathodes.

Reviewer 3:

The principal investigator (PI) has developed collaborations with national laboratories, universities, and industries, the reviewer noted.

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 the proposed work as a good combination of theoretical modeling and experimental approach to continue improving layered-layered-spinel cathode materials.

Reviewer 2:

Current work of stabilization using spinel structure should be vigorously continued in combination with doping studies, the reviewer urged, while recommending that work related to coatings other than atomic layer deposition (ALD) should be de-emphasized. That work will in general be merely a Band-Aid and a sheer waste of resources, the reviewer asserted. In the reviewer's opinion, if a fundamental solution is not found, such as by manipulation of the bulk structure as pursued here, coatings, as has historically been seen from massive past work at Argonne National Laboratory (ANL), will not save the day for this cathode system. In conclusion, the reviewer recommended the modeling work be pursued collaboratively with groups possessing greater expertise.

Reviewer 3:

The reviewer described the proposed future research as continuing development of these LLS cathodes to optimize their capacity and electrochemical stability, and expanding the materials characterization techniques, e.g., through Raman spectroscopy and augmenting them with modeling studies to understand the bulk and interfacial structures of these materials. It is, however, equally important, the reviewer said, to demonstrate the benefits of these LLS cathode materials in an industrial environment in comparison with the surface-treated NCA-based cathode to properly assess the technical barriers in the Vehicle Technologies Office (VTO).

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

Reviewer 1:

In the reviewer's estimation, this project has the highest relevance to the U.S. Department of Energy's (DOE) goal. In fact, the reviewer, elaborated, this is the only high-capacity cathode system that has any realistic chance of being deployed in the near future in automotive applications.

Reviewer 2:

The low specific energies and high costs of lithium (Li)-ion batteries are serious impediments to their widespread adoption in vehicles, the reviewer summarized, and high-capacity cathode materials are required to address these shortcomings. While LMR-LLC cathodes are promising from both energy and cost perspectives, the reviewer noted that they are hampered by issues such as voltage fade and hysteresis. Spinel embedded materials of this class, the reviewer speculated, may mitigate these issues, resulting in stable structures, as is being addressed in 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 recommended increasing project funding because this is the core program of the LL materials.

Reviewer 2:

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

High-Capacity, High-Voltage Cathode Materials for Lithium-Ion Batteries: Arumugam Manthiram (University of Texas at Austin) - es051

Presenter

Arumugam Manthiram, University of Texas at Austin.

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 praised the approach of exploring and characterizing vanadium (V)-based cathodes, especially from fundamental points of view, for the development of a higher-capacity cathode as an excellent idea. The reviewer acknowledged that it is high-risk work but said the effort to understand the structure/property relationship is of utmost importance to facilitate further studies.

Reviewer 2:

The reviewer remarked that the objective of this project is to develop new polyanion phosphate cathodes with high specific capacity for Li-ion batteries, exhibiting multi-electron redox process, and to gain a fundamental understanding of their structure/composition/performance relationships. The reviewer then enumerated the types of cathodes being developed; first, the three polymorphs of LiVOPO_4 , wherein two lithiums can intercalate; second, nanostructured phosphate cathodes with either graphene inclusions or aliovalent metal dopings for enhanced conductivities and performance. Low-temperature synthesis methods are being developed for these cathodes to improve their ionic and electronic transport, the reviewer continued. Although the approach looks well-designed and feasible, the reviewer said, with these different cathode materials – $\text{Li}_3\text{MCO}_3\text{PO}_4$, LiVOPO_4 and doped LiCoPO_4 – it looks a bit diffuse. It is debatable, in the reviewer's opinion, if these cathodes (especially LiVOPO_4) could be a promising candidate for high-energy cathodes, with its low intercalation potentials for second lithium.

Reviewer 3:

The reviewer found the approach weak in that proposed materials – nickel, cobalt and V – are scarce and expensive. The reviewer also considered that capacities for materials were measured at unrealistically low

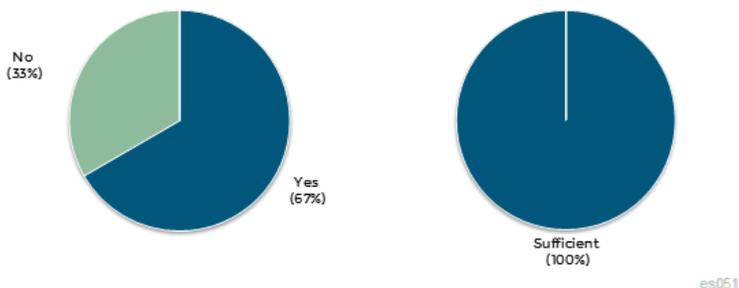
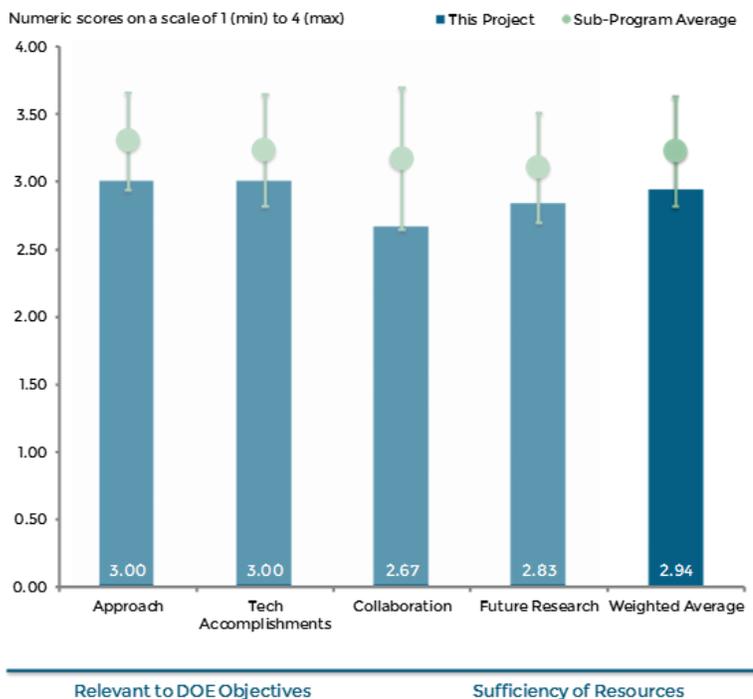


Figure 2-2 High-Capacity, High-Voltage Cathode Materials for Lithium-Ion Batteries: Arumugam Manthiram (University of Texas at Austin) - Electrochemical Energy Storage

rates. Should be C/3 as a minimum. The reviewer added that the potential for sodium intercalation may or may not be relevant to DOE 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 towards DOE goals.

Reviewer 1:

While the LiVOPO_4 cathodes did not turn out to be promising, the reviewer said, the work the authors have carried out is exhaustive (various synthetic procedures, materials engineering, characterization, etc.) and contributes to a solid understanding of their properties and potential thus expanding the technical database. The reviewer termed discovery of the new layered VOPO_4 as also interesting and wondered if, as the author suggested, it can act as a host for sodium (Na) or Mg insertion.

Reviewer 2:

Interesting studies were made on the LiVOPO_4 cathode in three different crystallographic forms, the reviewer noted, demonstrating intercalation of more than one Li and capacity greater than 200 mAh/g, albeit at low voltages for the second Li, also confirmed from chemical lithiation. The reviewer also found it interesting to note that an aliovalent substitution of V^{3+} for Co^{2+} decreases polarization and increases the initial capacity to approximately 100 mAh/g, even without carbon (C) coating. Finally, the reviewer observed, three polymorphs of LiCoPO_4 have been synthesized by a facile microwave method (yet to be characterized) and that these studies also led to some good publications. Although in the reviewer's opinion a good understanding has been gained from the low-temperature synthesis (and characterization) of these advanced cathodes, the performance characteristics of these materials do not compare well with the layered cathodes.

Reviewer 3:

The reviewer noted that the materials studied in this project offer no improvements over existing cathode materials and found it very hard to understand the overall strategy. It appeared to the reviewer to be a program of trial and error, albeit intelligent trial and error. However, the reviewer considered that the theory behind the approach sounds good. The material kinetics were measured only at very low rates, the reviewer said, and may be hard to improve. The best candidate materials still have many unresolved problems, the reviewer noted in conclusion.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

More collaborative effort would have been desirable, in the view of this reviewer.

Reviewer 2:

The reviewer discerned no formal collaboration in this project so far. Although the work is rather exploratory, the reviewer said, some collaboration with external partners would be helpful.

Reviewer 3:

Noting that only one collaboration had been shown in the presentation, the reviewer believed the project was very weak in this aspect.

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:

Focused efforts to manipulate the electronic properties using conductive agents and synthetic procedures are certainly the right future directions, the reviewer agreed. The reviewer suggested work using materials that will

have practical relevance, rather than focusing on high Co content compounds and cathodes with huge difference between the voltage plateaus, if any. On the other hand, the reviewer noted, work with Na and Mg could also be interesting.

Reviewer 2:

The reviewer described the proposed future research as to continue the development and study of the three polymorphs of LiVOPO_4 cathode and to down-select one for further study on the synthesis of LiVOPO_4 /graphene nanocomposites to improve conductivity and thus increase the capacity to about 250 mAh/g. Likewise, the reviewer continued, aliovalent doping of M (in LiMPO_4 ; M= iron (Fe), Mn or Co) with V_{3+} or Ti_{4+} will be explored to improve their ionic/electronic conductivities. The proposed materials look interesting, the reviewer said, but the approach seems to be truly exploratory and non-specific. Nor do the expected improvements appear to be significant compared to some of the known layered, mixed metal oxide materials (Ni-rich or even the surface-treated NCA cathodes), in the reviewer's opinion. This reviewer agreed with a suggestion offered by another, that there should be more focus on improving the cycle life and rate capability of the VOPO_4 cathodes or, more important, on exploring newer cathode materials that can intercalate multiple Li-ions and/or provide higher capacity.

Reviewer 3:

Seeing no overall strategy for material selection and evaluation, the reviewer said the project appeared to rely on a cut-and-try strategy.

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

Reviewer 1:

The low specific energies and high costs of Li-ion batteries are serious impediments to their widespread adoption in vehicles, the reviewer noted, thus, improvements in the specific energy of electrode materials will result in increased vehicle range and reduced battery cost. Because state-of-the-art cathode materials have low specific capacities due to intercalating only one Li per transition metal, the reviewer said, new cathode materials with an ability to intercalate multiple lithiums address this technical barrier.

Reviewer 2:

The search for alternative cathodes capable of multi-electron redox process is an important research topic to achieve significantly higher energy density cathodes, the reviewer observed, hence the topic is highly relevant.

Reviewer 3:

The reviewer expressed doubt that the project would result in any positive effect and found it unclear that any improved materials would be forthcoming.

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

Reviewer 1:

This reviewer considered the funding level sufficient because the project is exploratory research.

Reviewer 2:

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

Reviewer 3:

The third reviewer said it was not clear how project milestones and resources were related.

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

Presenter

Marca Doeff, Lawrence Berkeley National Laboratory.

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:

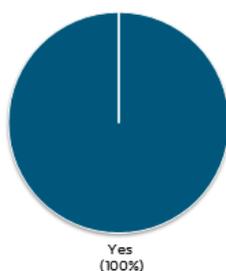
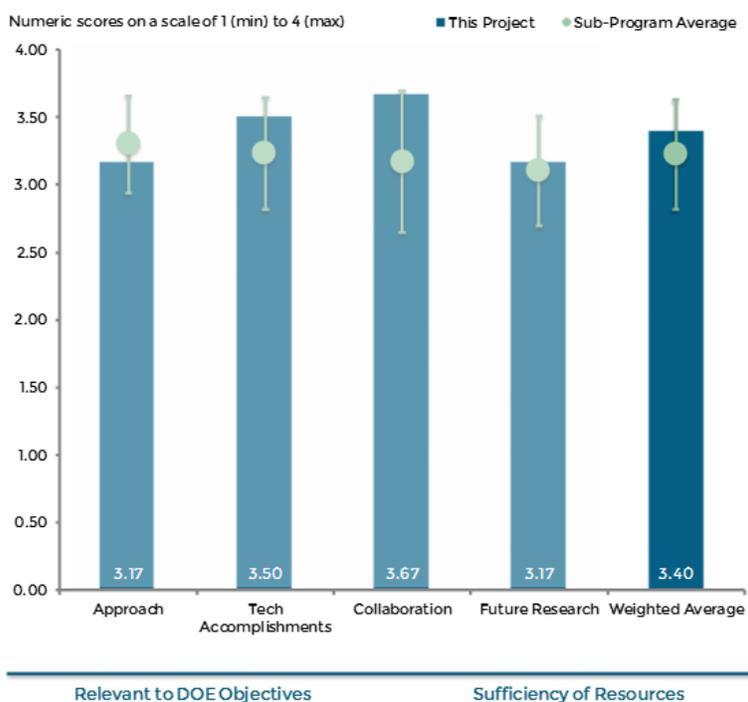
Partial Ti-substitution for nickel manganese cobalt oxide (NMCs) cathodes increases the capacity and cyclability, the reviewer observed.

Reviewer 2:

The reviewer found the work narrowly focused on only one dopant and expressed a desire to it expanded to include series of dopants such as those of different oxidation states, for example, and evaluate their impact. The reviewer also thought the work should have included NMC of different compositions.

Reviewer 3:

In previous years, the reviewer said, this project showed that the aliovalent substitution of NMC cathode materials with titanium (Ti) results in improved capacities and cycle life, especially at high charge voltage. The objective this year, the reviewer said, was to understand the beneficial effects of Ti substitution in terms of the bulk and interfacial properties using a suite of advanced analytical techniques (synchrotron); to further develop the spray pyrolysis method to synthesize the NMC cathodes in a single step to control the morphology (hollow particles); and to examine the possibility of affecting a surface coating on the cathode particles. Alternatively, the reviewer noted, surface coating was implemented using additional ALD/molecular layer deposition (MLD) coating. The strategy of altering the bulk and interfacial properties of the NMC cathodes through suitable substitutions is feasible, in the reviewer's opinion, although, the reviewer qualified, not as novel as was claimed in the presentation. With the hollow morphologies possible thus far, the reviewer said, spray pyrolysis, although appealing from a process standpoint, may not be acceptable in terms of tap densities. Finally, the reviewer speculated, overlaying another coating on the cathode material with desired surface layer (through Ti substitution) may offset the benefits of Ti substitution.



es052

Figure 2-3 Design of High-Performance, High-Energy Cathode Materials: Marca Doeff (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

Theoretical calculations have been verified with experiments, the reviewer observed.

Reviewer 2:

Although believing the studies were to some degree limited in scope, the reviewer complimented the authors for having done an excellent job in preparing and characterizing the materials, from both experimental and modeling points of view. The reviewer praised the results related to structural reconstruction during high-voltage cycling as very insightful and the conclusions as carefully drawn and well presented.

Reviewer 3:

Good progress has been made in understanding the compositional changes of the Ti-doped NMC cathodes both in the bulk and on the reconstructed surface layer, the reviewer said, noting that a few good publications have resulted from these studies. Some of the findings were, in the reviewer's opinion, quite expected; for example, that the surface reconstruction would occur in the first cycle and depend on the charge potentials. If the aliovalent Ti-substitution lowers the potential profile on discharge also, the reviewer remarked, that might offset the gain in capacity. Moreover, the reviewer continued, the longevity of Ti-substitution on the surface properties has yet to be established and the cycling data presented does not support the claim that the cycle life has improved. The reviewer noted noticeable capacity fade even with Ti-doped NMC. Finally, the reviewer wondered if the improved performance of the spray pyrolysis material might be due to higher surface area (hollow morphology). If so, the reviewer concluded that would imply increased electrolyte-affected degradation of the surface.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

This is an exemplary collaborative project, in the view of this reviewer.

Reviewer 2:

There is good collaboration with several researchers at Lawrence Berkeley National Laboratory (LBNL), the reviewer observed, as well as with external researchers, especially in carrying out the basic studies to understand the nature of the reconstructed surface layers. The reviewer raised the possibility that collaboration with an industrial partner could be useful to assess the benefits of this material in relation to several other NMC materials available within the industry.

Reviewer 3:

The PI has developed collaborations with many researchers at several national laboratories and universities, the reviewer noted.

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 research is reasonable and operable, in this reviewer's estimation.

Reviewer 2:

The authors should move away from fancy synthetic routes such as spray pyrolysis to prepare core-shell, hollow structures, the reviewer recommended, as these will invariably be more expensive to manufacture and offer no apparent benefit in performance (with lower density). The reviewer also suggested the project team

explore higher Ni content materials using dopants and study their thermal behavior – a key drawback of this group of cathode materials. Recognizing that it is tempting to look for multiple solutions, the reviewer encouraged the project team to remain focused on a few key items such as substitutions and de-emphasize “me too” types of work such as coatings.

Reviewer 3:

The proposed future work for the balance of the project duration is to explore the composite core-shell structures, if possible, from the spray pyrolysis and with suitable surface coatings, the reviewer observed. Future studies in a new, related project, the reviewer added, will include NMCs with higher Ni content NMC compositions and the synthesis of core-shell materials using spray pyrolyzed hollow spheres.

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

Reviewer 1:

The reviewer called the project very relevant, but believed that focusing on only one dopant limited its experimental scope.

Reviewer 2:

High-energy-density electrode materials are required to improve the specific energy of Li-ion cells and thus increase vehicle range and reduce battery cost, the reviewer said. The reviewer reiterated that state-of-the-art cathode materials provide capacities of only about 170 mAh/g, about half the capacities possible from the (C) anodes. There is a need explore new cathode materials, which this project is duly addressing, the reviewer concluded.

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

Reviewer 1:

The funding level seems right, said this reviewer.

Reviewer 2:

The reviewer assessed resources as being adequate for the scope of the project.

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

Presenter

Gerbrand Ceder, Massachusetts Institute of Technology.

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:

Seeking out new, high-energy-density positive electrode materials is a huge technical challenge, the reviewer said, adding that the PI is tackling this problem from mechanisms learned from predictive modeling.

Reviewer 2:

Noting that Li-excess, layered composite, transition metal oxide electrode materials are some of the most challenging material structures to study with first-principles calculations, the reviewer said the PI’s approach was excellent, while also claiming not to be the best judge of this type of work.

Reviewer 3:

The reviewer called this a very interesting blend of theoretical work with experimental and practical work where new compounds are used to test the theoretical suggestions, and noted that it is very focused on the critical barriers.

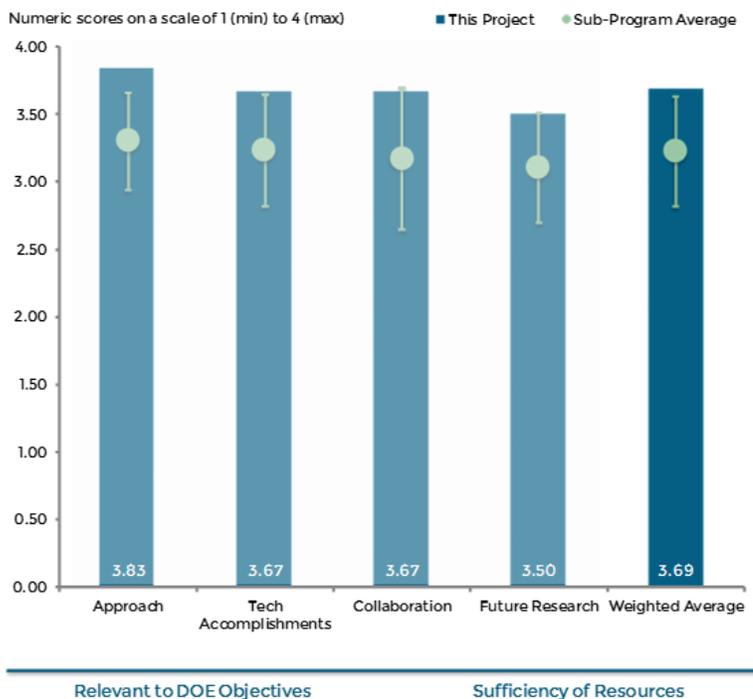
Question 2: Technical Accomplishments and Progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

Reviewer 1:

The insights gained in this project are providing guidance to material innovation, the reviewer stated.

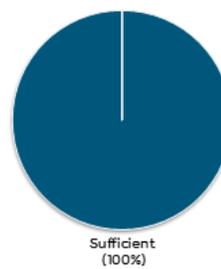
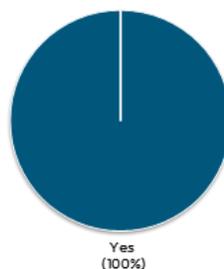
Reviewer 2:

The reviewer said the percolation concept the author found and later tested in practice is new and termed it a real accomplishment. Likewise, the reviewer found it very interesting to learn that a $\text{Li}(\text{Li},\text{Mn},\text{Nb})\text{O}_2$, with a



Relevant to DOE Objectives

Sufficiency of Resources



es054

Figure 2-4 First Principles Calculations of Existing and Novel Electrode Materials: Gerbrand Ceder (Massachusetts Institute of Technology) - Electrochemical Energy Storage

high degree of oxygen participation in the redox process, is a stable cathode material that does not fall apart as the electrode is cycled. The reviewer looked forward to hearing the mechanism behind this behavior explained in the future.

Reviewer 3:

While agreeing that the PI has done a significant amount of work and shown considerable progress, the reviewer was unclear on the PI's conclusion that over-lithiation should improve diffusion in these materials when the opposite is generally true. The reviewer also questioned some of the model compound choices, noting that, while they may be very interesting, they will never be in transportation-oriented batteries.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer remarked that the PI has a number of collaborations with other modelers and researchers examining these complex materials.

Reviewer 2:

Strong collaboration is clearly shown, the reviewer said, and, in particular, the strong correlation between theory and experimental results is very encouraging.

Reviewer 3:

Modeling and experiments are combined well in this project, 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 reviewer noted that the PI is planning to extend his present studies.

Reviewer 2:

The reviewer praised the establishment of the relationship of lattice expansion/contraction to diffusion as very insightful. It means, the reviewer went on, that there will be some strong coupling between stress and diffusion and because diffusion and concentration gradient will induce stress in the electrodes, the stress will in turn change diffusion. The reviewer wondered if strain engineering might provide another knob to tune the capacity and rate performance of the cathode materials. Also, the reviewer asked what the future development plan is for the new Li- excess materials, such as LMCO and $\text{Li}(\text{Ni}_{2/3}\text{Sb}_{1/3})\text{O}_2$.

Reviewer 3:

The area of oxygen participation in the redox process seemed to this reviewer to be very intriguing and in the reviewer's opinion, its relation to the oxygen loss is very important. If the authors managed to propose a mechanism for the loss of oxygen, that result, by itself, could be very useful, the reviewer predicted.

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

Reviewer 1:

This project will lead to improved high-energy-density oxide electrode materials, the reviewer predicted, which should reduce costs and enable further electrification of the nation's vehicles, resulting in improved gas mileage.

Reviewer 2:

Yes, the reviewer said, in particular when talking about high-capacity cathode powders which are, at the moment, the most important active ingredient limiting the overall capacity of the Li- ion battery.

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

Reviewer 1:

The PI is effectively using the available funds, the reviewer concluded.

Reviewer 2:

The resources are sufficient, the reviewer said, depending on how much experimental work is required.

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

Presenter

Clare Grey, University of Cambridge.

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 project team is using carbon 13 (C13) to understand the composition and change with time of solid electrolyte interface (SEI) components, the reviewer noted, terming it an extremely valuable approach and highly relevant. Dr. Grey uses multiple techniques and collaborations to understand what is happening at the atomic and molecular level, the reviewer observed, and focuses on understanding how these insights relate to macroscopic battery behavior.

Reviewer 2:

The reviewer believed it safe to say that the PI is the world leader in conducting nuclear magnetic resonance (NMR) studies on batteries, battery components, and battery materials, having proven such studies can provide insights into battery operation and degradation mechanisms. There are others the reviewer believed are in the PI's class, most of whom worked with the PI at some point. The approach to this work, the reviewer said, represents the quality of this group of researcher. The only aspect the reviewer would question is the breadth of studies conducted under this effort, which the reviewer noted is attacking a lot of very difficult problems.

Reviewer 3:

The reviewer observed that the project investigated the SEI composition of silicon (Si) and studied the effect of FEC and VC on composition. Li-ion conductivity in SEI should be investigated using NMR, and noted that no study on electrode tortuosity was reported.

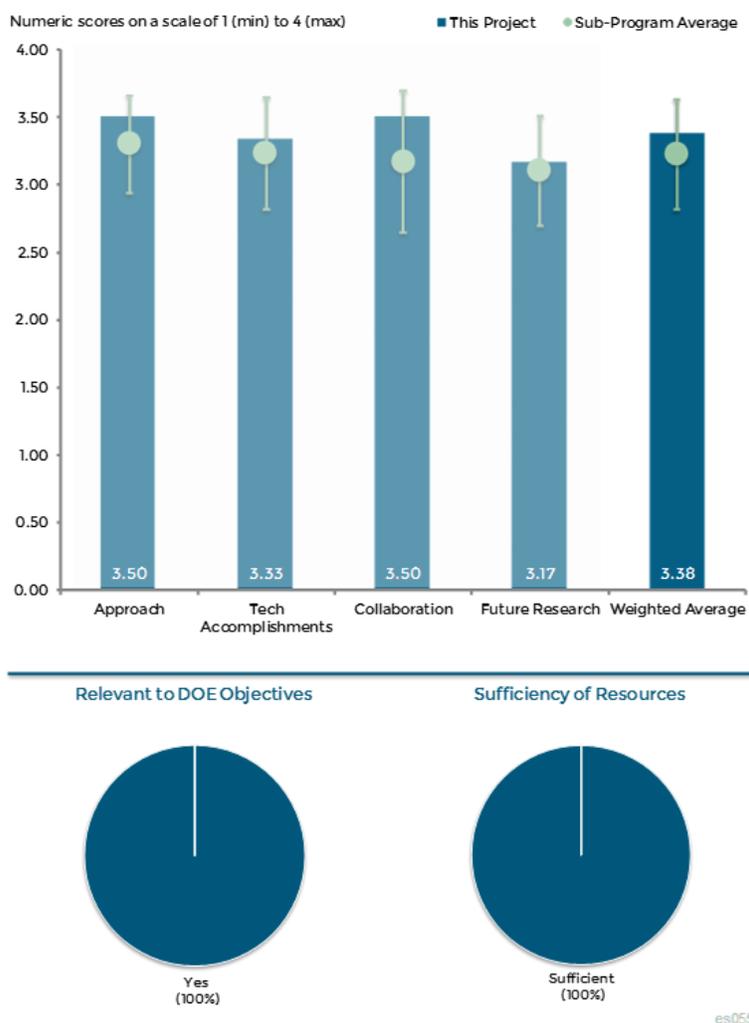


Figure 2-5 First-Principles Calculations and NMR Spectroscopy of Electrode Materials: Clare Grey (University of Cambridge) - - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

This reviewer praised excellent conclusions and progress, but was unsure concerning the point of the Na anode diagnostics. Another valuable focus to consider in the future, the reviewer suggested, would be attempting to gather evidence for whether Si SEI is stable at a constant Voltage. Does the film passivate, the reviewer asked, or does it continue to grow, consuming Li and electrolyte components, even when the anode is held at a constant voltage (i.e., not cycled).

Reviewer 2:

The reviewer noted that the focus of the presentation was on the silicon electrode, and that work is also being conducted on other advanced battery chemistries. The reviewer did not always agree with the PI's conclusions, citing in particular the explanation of the hysteresis in Si cycling. Nevertheless, the reviewer applauded the fact that suggestions were offered concerning phenomena and mechanisms observed in these studies.

Reviewer 3:

The use of NMR to study the mechanism of Li-S is unique and innovative, the reviewer said, noting that the results were published in the Journal of the American Chemical Society (JACS), a top technical publication. But the reviewer perceived the research lacked focus.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The PI has extensive collaborations in the United States and around the world, the reviewer observed.

Reviewer 2:

The PI, the reviewer noted, has always focused on understanding the most relevant issues affecting a battery issue, and uses extensive collaborations to do that. Nine institutions were listed as collaborators, many with more than one researcher, the reviewer remarked, terming this excellent.

Reviewer 3:

The project has collaborated closely with several PIs to obtain Si nanowires, SEI and additives, 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 reviewer described the future planned work as very ambitious.

Reviewer 2:

The Si SEI work is excellent and highly relevant, the reviewer said, referring to earlier comments on whether the Si SEI is truly passivating. Another valuable focus, in this reviewer's opinion, would be trying to understand the effect of additives, such as FEC, on the SEI makeup. The reviewer was unsure about the purpose of the Na dendrite study, because Na offers no obvious benefit for transportation applications, in the reviewer's view.

Reviewer 3:

The reviewer suggested future work include study of Li-ion conductivity in SEI.

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

Reviewer 1:

This project, the reviewer predicted, will lead to improved Li-ion and succeeding battery technologies, which should reduce costs and enable further electrification of the nation's vehicles, resulting in improved gas mileage.

Reviewer 2:

Referring to earlier comments, the reviewer deemed Si SEI understanding excellent.

Reviewer 3:

SEI is very important for cycling stability of Li-ion batteries, the reviewer opined.

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

Reviewer 1:

The project has accomplished a tremendous amount of work and progress for a relatively small amount of funding, this reviewer said, adding a willingness to support further funding if that were requested.

Reviewer 2:

The reviewer described the PI as very productive and teaming with many colleagues.

Reviewer 3:

The PI has sufficient resources for the project, in the view of this reviewer.

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

Presenter

Jason Zhang, Pacific Northwest National Laboratory.

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 approach to understanding the behavior of Li_2MnO_3 in order to improve the voltage fade issue of LL cathode is a good one, the reviewer agreed, and the analytical tools employed were also very effective and complementary. The reviewer believed that the coating work did not have to be included, calling it kind of run-of-the-mill work.

Reviewer 2:

The reviewer described the objective of the project as being to understand the structural aspects and mechanisms contributing to capacity loss and voltage fade of LMR-LLC cathode materials and minimizing these processes by developing suitable surface coatings on the cathode materials. Additionally, low-cost synthetic methods for cathode materials were pursued. This project thus addresses one of the key performance barriers of LMR-LLC cathodes, adopts a viable approach and is well integrated with other efforts in understanding and mitigating voltage fade. However, the reviewer noted some elements that overlapped strongly with efforts on the same type of LMR-LLC cathodes or NMC cathodes, citing characterization of the surface layer as a disordered rock salt structure and noting its similarity to the reconstructed surface layer studies done at Lawrence Berkeley National Laboratory (LBNL). Further, the study of the aluminum fluoride (AlF_3) surface coating overlaps with efforts at ANL, the reviewer added, albeit with a different conclusion, namely that the surface coating reduces voltage fade – an apparent inconsistency with the overall program point of view. Finally, the reviewer regarded the focus on high-voltage operation of traditional NMC cathodes with 180 mAh/g somewhat unrelated.

Reviewer 3:

The reviewer recommended that targets should include maximizing use of low-cost materials and that use of cobalt and nickel needs be minimized. It was unclear to the reviewer what the overall technical goals were in a

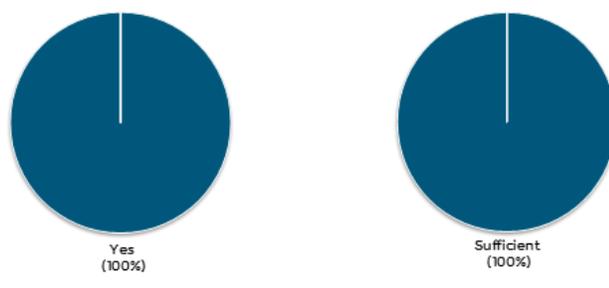
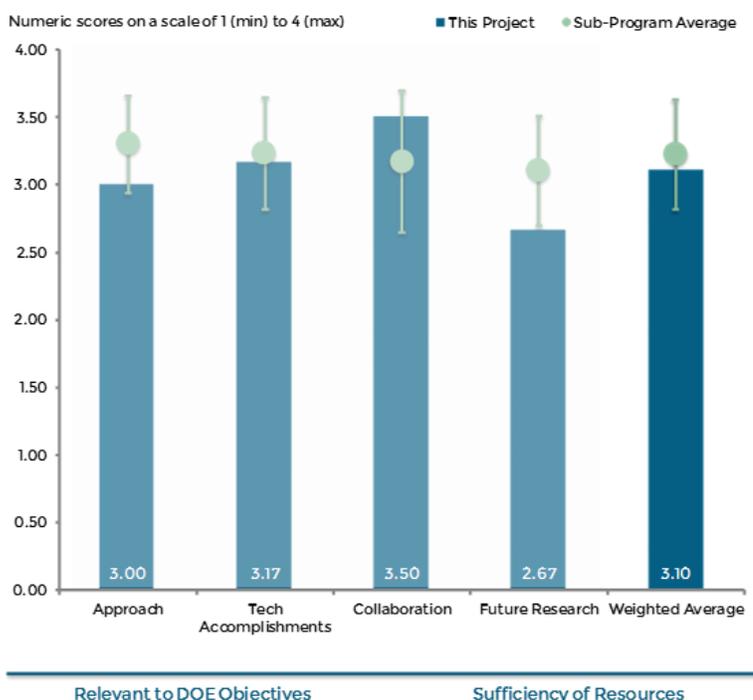


Figure 2-6 Development of High-Energy Cathode Materials: Jason Zhang (Pacific Northwest National Laboratory) - Electrochemical Energy Storage

quantitative statement. While fundamental studies are a good idea, in the reviewer's opinion, general improvement is not a technical goal.

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 towards DOE goals.

Reviewer 1:

The team has done an excellent job in characterizing the behavior of Li_2MnO_3 during initial charging and subsequent cycling, the reviewer said, and data related to TM ion migration, structural change, effects of oxygen non-stoichiometry are also of high quality. The reviewer regarded the effects of coating as minimal and some of the cycling result-based statements as too preliminary to be highlighted.

Reviewer 2:

Good progress has been made in understanding phase transformations in a LMR-LLC cathode on cycling to a defect spinel and ultimately to a disordered, rock-salt structure, the reviewer noted, which is attributed to voltage fade. Such transformation is shown to be minimized by a surface coating of AlF_3 by reducing electrolyte-induced degradation. The reviewer also remarked on several good publications resulting from these studies. The reviewer considered these results interesting, observed that they imply the pseudo-spinel transformation of the LMR-LLC cathodes is surface-related, which is not consistent with observations by ANL and others. Phase transformation is more bulk phenomenon, the reviewer said, and cannot be controlled through surface modifications (coating). The study on oxygen non-stoichiometry to facilitate Li_2MnO_3 component appeared to the reviewer to accelerate voltage-fade degradation. Hydrothermal synthesis appears to provide slightly better performance, the reviewer noted, but recommended the comparison be made with materials of similar tap densities and of similar loadings. The cycle life data of the LMR-LLC cathodes the reviewer in general found impressive, but the loadings are still quite low (4 mg/cm^2), compared to the levels required in high-energy Li-ion cells. Unlike conventional cathodes, the reviewer said, performance of LMR-LLC cathodes depends strongly on the loading because of poor kinetics.

Reviewer 3:

Some improvements in performance and life have been achieved with coating technology, the reviewer remarked, but other improvements are a wash. Fundamental understanding should lead to more positive technical results, the reviewer said. Full control of phase transition from spinel to rock salt was not achieved, the reviewer noted, and bulk material properties were not modified.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

An excellent collaborative effort that also resulted in good, high-quality data, in the view of this reviewer.

Reviewer 2:

There are good collaborations with several researchers within DOE and elsewhere, the reviewer said, suggesting it is probably the appropriate time to collaborate with a battery manufacturer to assess the performance of these modified (hydrothermal assisted [HA] and coated) materials.

Reviewer 3:

The reviewer discerned good collaboration with the appropriate expertise at other institutions which supply needed 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:

The reviewer noted that the current project will end in a few months, at which time the focus will apparently shift to traditional (non-Li-rich) NMC cathodes to investigate the interface and bulk properties of both pristine and cycled cathode using advanced characterization techniques (especially operando TEM using liquid electrolyte). The objective will be to achieve high capacities of 200 mAh/g or more at high charge voltages and enhance the cyclic stability of such materials.

Reviewer 2:

The reviewer expressed approval of the overall goal but described the work plan as rather generic to improve on the high-voltage, high-capacity performance of NCM materials and asked what specific lessons (e.g., synthetic) learned from current research results will be applied in future work to tailor the properties of NCM cathodes so they it can be cycled effectively. A question also posed by the reviewer was what NCM compositions the project team is targeting. The reviewer observed that 200 mAh/g was cited as a goal, which means the material will invariably be Ni-rich. This, the reviewer said, is a tough problem to solve, not only from the cycling standpoint but also from the point of view of safety. The reviewer asked what specific ideas the project team have to resolve these issues and suggested the team select a high-payoff approach and pursue it exhaustively.

Reviewer 3:

The project does not have a clear end strategy growing out of results achieved to date (which the reviewer characterized as very modest), and, in the reviewer's estimation, needs to be more successful in terms of achieving performance and life.

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

Reviewer 1:

Yes, it does support DOE's goal, the reviewer said, as it addresses the improvement of capacity and stability of high-energy cathodes that are the bottlenecks for higher-energy cells.

Reviewer 2:

Low specific energies and high costs of Li-ion batteries are serious impediments to their widespread adoption in vehicles, the reviewer observed, and while LMR-LLC cathode materials are promising from energy and cost perspectives, they are hampered by issues such as capacity and voltage faced upon cycling. It is essential, the reviewer concluded, to improve the cycle life of these high-energy materials to make them suitable for EV applications, as is being done in this project.

Reviewer 3:

The project has to be more successful in achieving high performance and life from new materials, in this reviewer's opinion.

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

Reviewer 1:

The funding level is sufficient, the reviewer reaffirmed.

Reviewer 2:

The resources are adequate for the scope of the project, said the reviewer.

Reviewer 3:

The reviewer found it very difficult to tell how resources and milestones are related.

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

Presenter

Xiao-Qing Yang, Brookhaven National Laboratory.

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 lauded in situ and ex situ x-ray diagnostic techniques as tremendously valuable for understanding the structural changes that battery materials undergo both during cycling and under abuse conditions.

Reviewer 2:

A set of characterization tools including the time-resolved X-ray diffraction (TR-XRD), mass spectroscopy (MS), in-situ XRD and X-ray absorption spectroscopy (XAS), high-resolution transmission electron microscopy (HR-TEM) are used to study the crystal structure, electronic structure and chemical structure, the reviewer observed, predicting that these unique analytical techniques will enable better understanding of the underlying mechanism of thermal stability of metal oxide cathodes in the Li batteries.

Reviewer 3:

The goal of in-situ diagnostic techniques is appropriate, the reviewer agreed, but pointed out that the XAS, XRD and TEM cannot be done without highly specialized equipment and thus are unlikely to assist the average manufacturing operation without serious investment. Accordingly, the reviewer went on, there must be a clear linkage back to operational parameters, which has not been done. This had the effect of making the research appear quite academic to the reviewer, when in reality it could be quite applicable. The approach and milestones line up to each other, the reviewer said, but not to the stated relevance and project objectives. The broader impact of this work was not clear to the reviewer, who summarized by calling it is interesting research that is being judged against inappropriate criteria at its own behest.

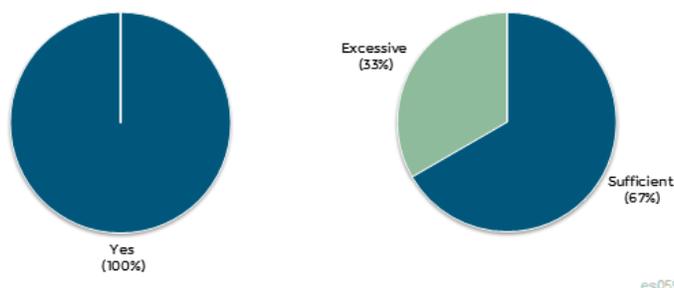
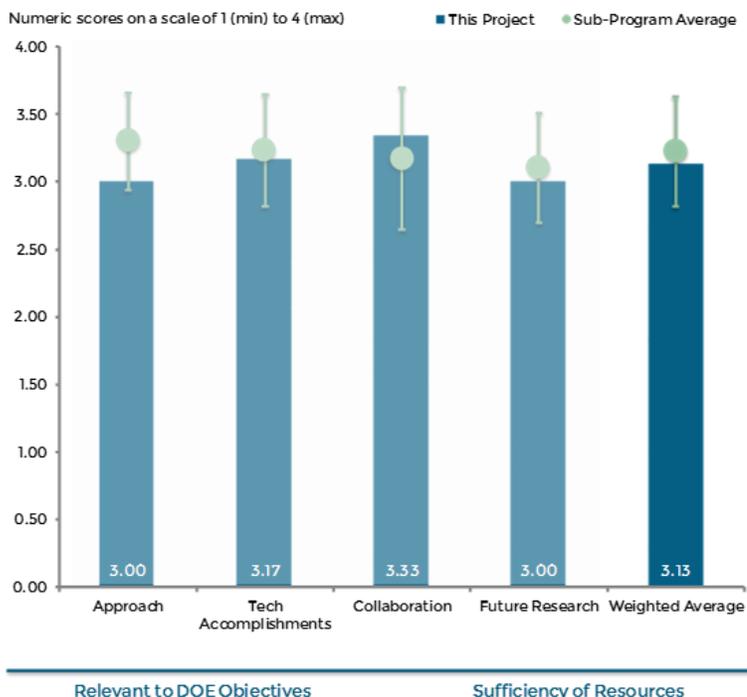


Figure 2-7 Advanced In-Situ Diagnostic Techniques for Battery Materials: Xiao-Qing Yang (Brookhaven National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The project has shown reasonably good progress, the reviewer said.

Reviewer 2:

A new unit-cell-breathing mechanism for Li_2MoO_3 during charge-discharge has been discovered using the synchrotron-based XRD, XAS and STEM and the corresponding results published in a prestigious journal, the reviewer recounted. Blended LiMn_2O_4 (LMO)- $\text{LiNi}_{1/3}\text{Co}_{1/3}\text{Mn}_{1/3}\text{O}_2$ (NCM) cathode materials with different stoichiometric ratios have been studied. The discovered specific physicochemical processes in the LMO and NCM should be described clearly in the annual report, the reviewer urged.

Reviewer 3:

The authors, the reviewer observed, have been prolific publishers, which reflects that their progress has been well recognized by their peers. The reviewer found the work and graphics quite interesting and potentially impactful. The concern expressed in an earlier comment, the reviewer said, was largely related to messaging, and not intended as an indictment of great research. The analysis of unit cell breathing is quite extraordinary, the reviewer said, predicting it could potentially lead to great insights in the design of future battery technologies. In the reviewer's opinion, the key element in the characterization is offering advice to the general battery community on how to produce better cathodes (LiNiMnO_4), but as this project nears completion it was not clear that this key outcome is being prioritized.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The results coming out of this project have benefited from the extensive collaboration network built by the PI, said the reviewer.

Reviewer 2:

The loss of key equipment at Brookhaven has led to a number of fruitful collaborations with laboratories and partners around the country, the reviewer observed, and the work has also engaged industry partners, which is key to transitioning diagnostic techniques out of the lab. Active engagement of the broader battery community is a key strong point of this work, in the opinion of this reviewer.

Reviewer 3:

While the reviewer saw evidence of a lot of collaboration, there appeared to be none with any of the groups supporting DOE VTO to develop high-energy batteries for automobiles. The reviewer recommended much more collaboration with other national laboratories, universities and battery companies working on novel materials or cells that meet DOE electric vehicle (EV) or plug-in hybrid electric (PHEV) goals.

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 recognized that providing guidance is called out in the fiscal year (FY) 2016 proposed work, which the reviewer views as critical to project success. To have a meaningful impact, the reviewer continued, the work must rationally influence process design. Likewise, the reviewer recognized that this work is a natural continuation of ongoing work, but was critical of its apparent academic bent. To ensure that it has an appropriate impact, the reviewer asserted that there needs to be a focus applied after the proposed work.

Reviewer 2:

Several critical issues have been proposed by the research team, the reviewer noted. For example, the X-ray absorption near-edge structure (XANES) and the extended x-ray absorption fine structure (EXAFS) will be used to study the Mo K-edge of Li_2MoO_3 at different charge-discharge states. The transmission x-ray microscopy technique will be developed to investigate the three-dimensional element mapping of layer-structured cathode materials in the Li-ion battery research. The electronic structure and crystal structure at the atomic local range and long range of cathode material remain unclear, the reviewer observed, but if successful, the proposed future research will fill the critical knowledge gap in this field.

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

Reviewer 1:

Predicting that deployment of high-voltage cathodes will be critical to increasing the power and energy densities of battery packs, the reviewer said this work should aid in this process of electrifying vehicle transportation.

Reviewer 2:

The reviewer foresaw that the fundamental knowledge obtained will provide the guidelines for designing cathode material of Li-ion batteries and called the ongoing research well aligned with the mission and the objective of DOE's program.

Reviewer 3:

The reviewer failed to see much relevance in the work on Li_2MoO_3 . Although its theoretical capacity is high, molybdenum is not particularly abundant, and its reaction potential is quite low.

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

Reviewer 1:

Acknowledging that the diagnostic tests are particularly time-consuming, the reviewer found the lack of a key focus on impactful conclusions for this amount of money disheartening.

Development of Novel Electrolytes and Catalysts for Li-Air Batteries: Khalil Amine (Argonne National Laboratory) - es066

Presenter

Khalil Amine, Argonne National Laboratory.

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 project team is employing a good approach for developing catalyst and electrolyte for Li-air battery, in the view of this reviewer.

Reviewer 2:

The investigators adopted a creative approach to use the simulation design first, then with experimental testing, the reviewer observed, and its efficiency and effectiveness were demonstrated in their catalyst, electrode and electrolyte investigation for Li-air batteries.

Reviewer 3:

A very well-designed project focused on delivering timely results, said 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 towards DOE goals.

Reviewer 1:

A few good electrolyte and electrode structures (including catalyst) were investigated and good performance was demonstrated toward the project goals with all the milestones are successfully reached, the reviewer summarized.

Reviewer 2:

All tasks are on schedule and good use has been made of the theoretical and experimental tools, said the reviewer.

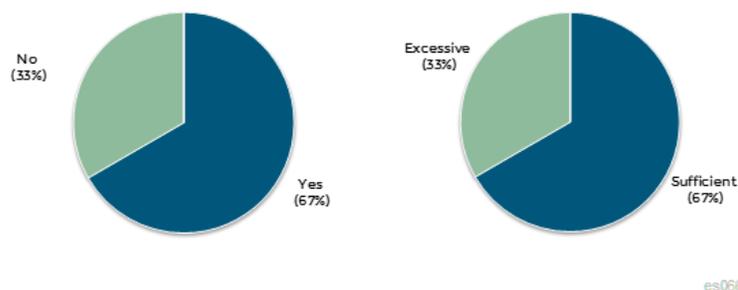
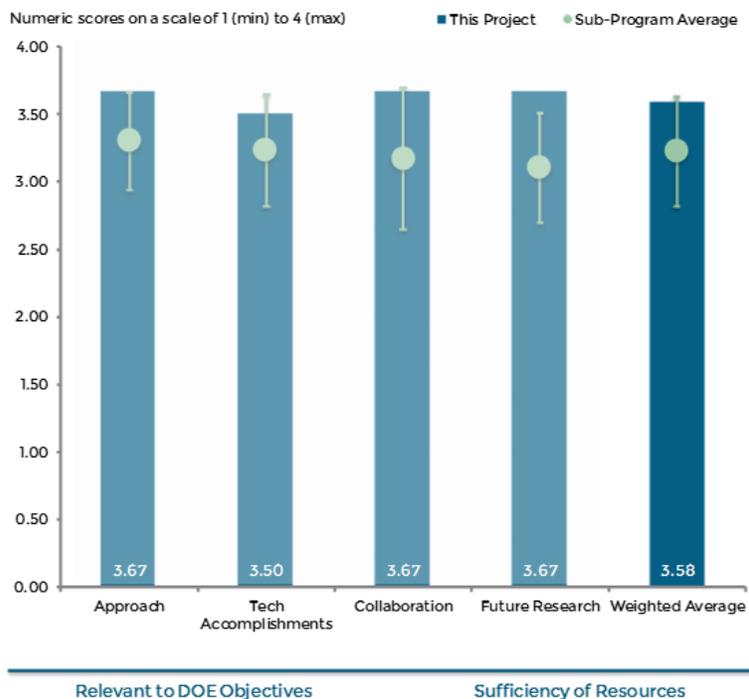


Figure 2-8 Development of Novel Electrolytes and Catalysts for Li-Air Batteries: Khalil Amine (Argonne National Laboratory) - Electrochemical Energy Storage

Reviewer 3:

Palladium (Pd) and molybdenum carbide (Mo₂C) catalysts are expensive, the reviewer observed, recommending that cheaper alternatives be developed and the result be demonstrated in a full cell configuration.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer cited good interaction and collaboration.

Reviewer 2:

The PI established wide international collaboration ranging from universities to national laboratories, the reviewer said.

Reviewer 3:

The results and the use of the characterization tools speak highly of the team, the reviewer commented.

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 research is solid and based on current achievements, the reviewer said.

Reviewer 2:

Proposed future work is focused on the results and data interpretation of work conducted to date, the reviewer said.

Reviewer 3:

Noting that development of new electrolytes and cathodes was proposed, the reviewer saw no strategy explained for developing materials nor what sort of materials were envisioned.

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

Reviewer 1:

The reviewer said reduce use of petroleum.

Reviewer 2:

The research for Li-air is in line with the objective of reaching high energy-density batteries to replace petroleum in vehicles, according to the reviewer.

Reviewer 3:

The recent DOE publications clearly state the fundamental limitations of the Li-air system that do not have clear solutions, the reviewer observed, which makes it important to support high- performing teams like this one to continue the search for new approaches.

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

Reviewer 1:

The PI has adequate resources to achieve the milestones and goals of the proposed project, this reviewer said.

Reviewer 2:

The reviewer praised both the team and their access to characterization tools as excellent.

Design and Scalable Assembly of High-Density Low-Tortuosity Electrodes: Yet-Ming Chiang (Massachusetts Institute of Technology) - es071

Presenter

Yet-Ming Chiang, Massachusetts Institute of Technology.

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 objective, the reviewer explained, is to develop a high-density, binder-free, low-tortuosity electrode using two approaches: directional freezing and magnetic alignment. Two alternative methods, sintered and non-sintered, are used for directional freezing. Sacrificial solids and emulsion chaining are investigated for magnetic alignment. The electrode tortuosity can be adjusted by these fabrication methods over a certain range. Low tortuosity electrodes appear to have better high-rate performance. Remaining challenges and barriers have been correctly identified, the reviewer said, and the proposed future work is well-planned and feasible.

Reviewer 2:

The technical approach is excellent in addressing the technical barriers to increase usable area capacity, the reviewer said.

Reviewer 3:

The reviewer believed that some aspects of the approach are very good and quite innovative, but found it difficult to see how any of the techniques being developed could be carried out at high speeds in a cost-effective manner, especially when compared to the current method of making electrodes. The reviewer expressed a secondary concern about the magnetic alignment technique because it leaves an iron contaminant that may cause problems during battery cycling.

Reviewer 4:

The target of thicker, high-performing electrode structures is an important one from a cost perspective, the reviewer said, and the concepts utilized are unique and interesting. However, unfortunately the reviewer found

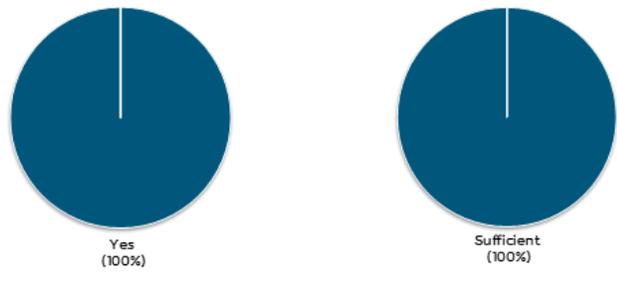
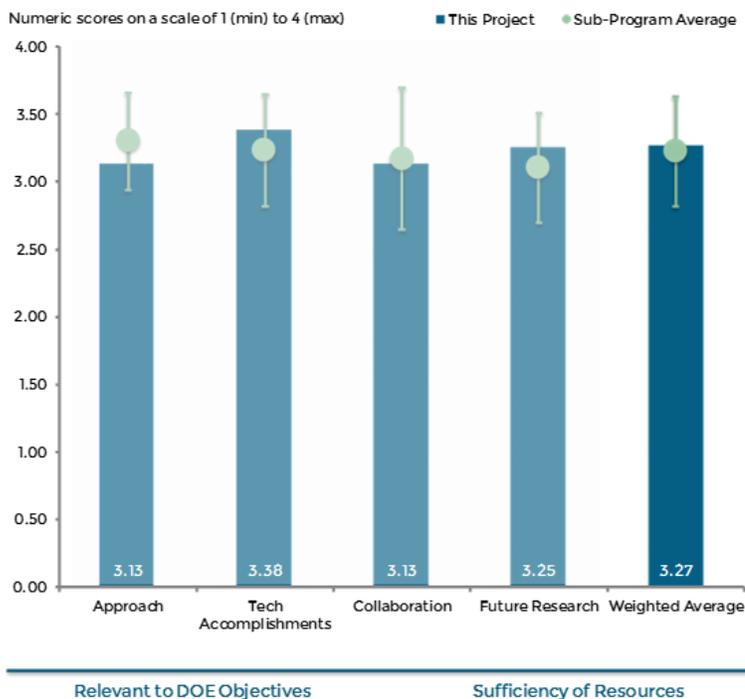


Figure 2-9 Design and Scalable Assembly of High-Density Low-Tortuosity Electrodes: Yet-Ming Chiang (Massachusetts Institute of Technology) - Electrochemical Energy Storage

it difficult to determine whether the cost advantage could be attained with either rather complicated process technology at a commercial scale.

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 towards DOE goals.

Reviewer 1:

Good progress has been made to the PI's goals, including some very good diagnostic studies, in the reviewer's opinion.

Reviewer 2:

It will be interesting, the reviewer said, to see the stability of the porous matrix during cycling at higher temperatures.

Reviewer 3:

The reviewer expressed a desire to have seen the performance characterization done against control electrodes of the same loading and made with traditional methods. The reviewer found it difficult to determine absolute levels of progress from the current data presented.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Collaborations appeared to the reviewer to be highly effective, particularly in introducing novel electrode fabrication methods such as the magnetic alignment approach.

Reviewer 2:

The PI has limited collaboration in the fabrication area, where support is needed, in the reviewer's estimation.

Reviewer 3:

Collaboration is minimal, the reviewer perceived, which was perhaps justified at such an early stage of development.

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 considered that, generally, the overall plan is good but expressed concern that one of the big problems with these three-dimensional architecture electrodes is attaching the electrode to the current collector, which has yet to be addressed.

Reviewer 2:

The reviewer hazarded that the PI may address several questions the review panel members and the general audience raised at the end of the presentation, such as how to attach electrodes made by directional freezing and magnetic alignment to the conductor; electrical field singularities at the pore openings; scaling laws for heat and mass transfer; and viscosity effects on the electrode microstructure and thickness.

Reviewer 3:

Finding the technical goals satisfactory, the reviewer suggested it could be valuable to begin to assess certain commercial attributes before the research gets too far advanced. These could include issues of cost, robustness etc.

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

Reviewer 1:

This project will lead to more optimized electrode microstructures, the reviewer predicted, improving both the energy efficiency and the cycle life of batteries. Ultimately, this could lead to reduced battery costs enabling further electrification of the nation's vehicles and improved gas mileage.

Reviewer 2:

This project directly supports fulfilment of DOE objectives, the reviewer said.

Reviewer 3:

Referring to earlier remarks, the reviewer said that, essentially, thick, high-performance electrode structures could be a significant boost to cost-effective designs.

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

Reviewer 1:

The PI has sufficient funds to meet his goals, the reviewer said, but the project will likely need further funding if it is worthy of bringing to production.

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

Presenter

Robert Kostecki, Lawrence Berkeley National Laboratory.

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:

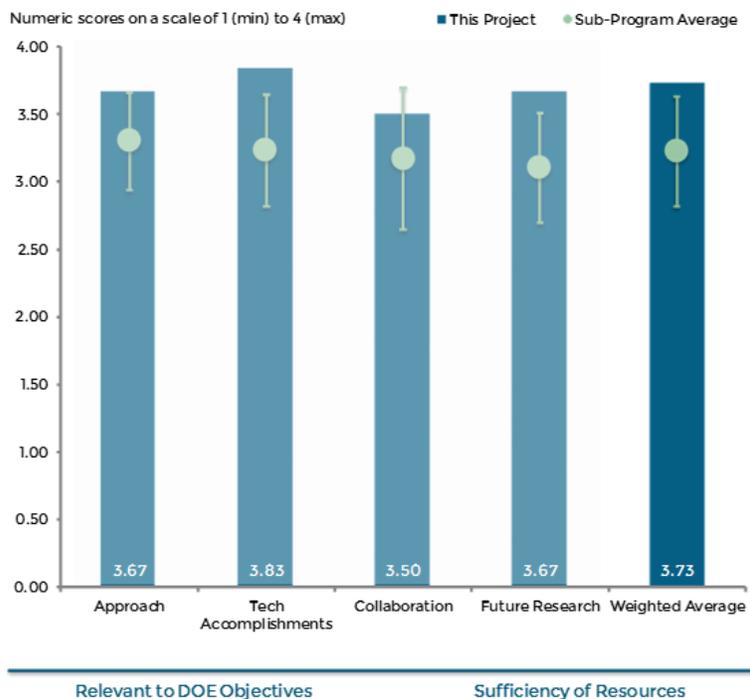
Use of in situ and ex situ Raman, fluorescence, Fourier transform infrared (FTIR), x-ray absorption spectroscopy/microscopy to study the capacity decay mechanism is critical to achieving long cycle life for Li-ion batteries, the reviewer opined.

Reviewer 2:

On the subject of metal dissolution from high-voltage cathodes, the reviewer noted that X-ray absorption, fluorescence spectroscopy and Raman spectroscopy have been used to identify compounds that form during cycling of cathode materials and said that gaining this knowledge is critically important for suppressing degradation of cells based on LMNO and NCM cathodes and Li, graphite and Si anodes. While not unique, the reviewer said, it is clearly very solid and has been found to be very successful for this study. The reviewer also noted that the project includes in-situ study of the surface coating on Si anodes and Li salts on SEI formation on Si using FTIR.

Reviewer 3:

Using diagnostic techniques to understand interfacial processes and structures is excellent, the reviewer said, and the PI uses a large number of advanced diagnostic techniques to provide insight into what is happening at battery interfaces. The reviewer questioned the value of fluorescence, as it is so general, providing very little quantitative information about interfacial species or even their abundance.



es085

Figure 2-10 Interfacial Processes in EES Systems Advanced Diagnostics: Robert Kostecki (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer noted the interesting result about the cause of impedance rise at the anode in Mn cathode-containing cells. It would be interesting to see, the reviewer said, if the use of electrolytes without carbonate esters results in a significant reduction in impedance rise at high temperatures in Mn cathode-containing cells. A next step here that would be very welcome in the battery community, the review stated, is a proposal for mitigating or eliminating this impedance rise mechanism. The reviewer was enthusiastic about the use of laser induced breakdown spectroscopy (LIBS) to study and understand the Si SEI and expressed interest in seeing how the Si SEI changes as the material is held at a constant voltage for varying lengths of time, to determine if the Si SEI is passivating and, if not, how the film changes with time, if at all.

Reviewer 2:

The formation of β -diketones ligands and metal complexes is an important finding, which explains the shuttle reaction from cathode to anode and dissolution of transition metals in cathode, the reviewer said. The new findings open a new opportunity to improve the cycling stability of Li-ion battery cells.

Reviewer 3:

Unique insights on compounds formed during transition metal dissolution have been identified and the mechanisms of their formation have been proposed based on the combination of experimental and modeling techniques, the reviewer noted. The formation of beta-diketones ligands and transition metal complexes has been explained and their impact on SEI formation and cell performance has been proposed. Insoluble metal complexes formed on the cathode surface may form a potentially insulating film, and the reviewer felt it would be desirable to characterize the conductivity of such a film in the future. A second possibility is that soluble metal complexes may migrate and damage the SEI and/or impede Li transport within the SEI. Here, the reviewer expressed a desire to see a future study of the possible degradation routes in the future. The reviewer considered that the project results to date have been quite outstanding. Gaining this critically important understanding, the reviewer predicted, will have a major impact on stabilizing transition metal oxide cathodes in Li ion batteries. Si SEI composition studies resulted in some insights, although some of these have been suggested previously and discussed by others. The reviewer summarized the project's findings by noting that lithium bisoxalato borate (LiBOB) addition to the electrolyte was suggested to promote oligomer/polymer SEI formation on the Si surface, which slows down SEI growth. And that neither nanoscale distribution of the components within the SEI nor SEI thickness is uniform. SEI was found to depend on the local Si/coating structure and morphology (e.g., aluminum alkoxide coating promotes formation of more organic components within SEI). It would be nice, the reviewer said, to gain more insights in the future on why different coatings had such impacts.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

LBNL has a large number of extensive collaborations with universities, other national laboratories, and battery companies, the reviewer stated.

Reviewer 2:

The PI has collaborated with multiple PIs in this program including the scientists at LBNL, ANL, NREL, etc., the reviewer noted.

Reviewer 3:

Multiple international and national collaborations have been successfully established, but the coordination within the collaborative network has not been spelled out clearly, in the view of this 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:

Calling the future research logically outlined and focused on overcoming critical barriers, the reviewer expressed a keen personal interest in learning more about the properties of the films formed on the cathode, the exact mechanisms of SEI damage by the metal complexes and why the SEI composition is strongly affected by the anode surface structure, morphology and composition.

Reviewer 2:

The reviewer expressed support for the move to understand high voltage stability in Ni-rich NMCs and encouraged the PI to confer with U.S.-based battery manufacturers, as many of them are also moving much of their focus to Ni-rich NMCs cathodes.

Reviewer 3:

The reviewer suggested studying the effect of Me (β -diketone) complexes on the conductivity (ionic/electronic) of SEI layers, on both anodes and cathodes.

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

Reviewer 1:

The mechanism of capacity decay for cathode and anode in Li-ion batteries is a critical to develop long-cycle-life Li-ion batteries, the reviewer said.

Reviewer 2:

The successful use of high-capacity materials will contribute to the reduction of Li ion battery cost, which should further promote electric vehicles on the road to replace regular gasoline-engine-powered vehicles, the reviewer stated, making this project absolutely supportive of DOE's goal.

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

Reviewer 1:

LBNL has enough resources to conduct proposed future research, the reviewer commented.

Reviewer 2:

The resources are adequate, the reviewer reiterated.

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

Presenter

Kristin Persson, Lawrence Berkeley National Laboratory.

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 approach is clear and focused and studying the structure and stability of the Li_2MnO compound as Li is removed from the structure is the right approach, the reviewer agreed, and is giving additional information about the voltage fade mechanism.

Reviewer 2:

This work is focused on understanding the voltage decay of a promising high-capacity cathode material via predictive modeling, the reviewer observed.

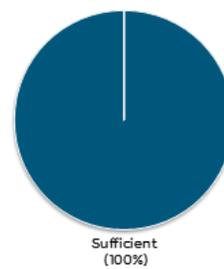
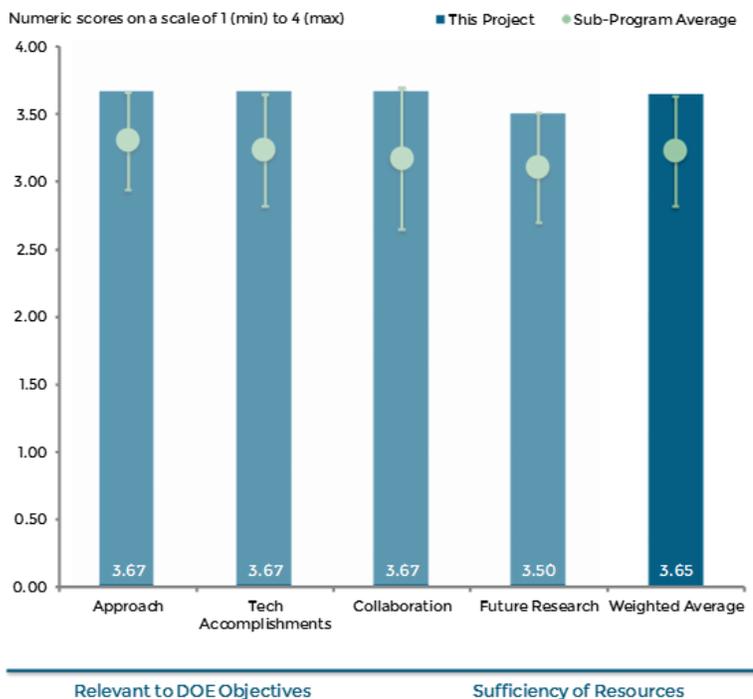
Reviewer 3:

The LMR-NMC electrode materials are some of the most challenging material structures to study with first-principles calculations, the reviewer remarked, and as one of the end members of the composite structure, Li_2MnO_3 is quite relevant. While disclaiming specific expertise in the area, the reviewer called the PI’s approach very good. However, the reviewer added, the literature indicates that Li_2MnO_3 domains within the composite structure cycle quite differently from the bulk material. Thus, extending this work to the actual composite structure may be a challenge.

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 towards DOE goals.

Reviewer 1:

The project team have produced extensive results on the cycling of the Li_2MnO_3 active material, the reviewer noted.



es091

Figure 2-11 Predicting and Understanding Novel Electrode Materials from First Principles: Kristin Persson (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer found the plots showing the stability of the Li_2MnO_3 structure moving toward a structure wherein Mn is displaced into the Li layer compelling and called the different kinetic behavior toward oxygen release between a surface oxygen and oxygen in the bulk very interesting. At some point, the reviewer said, it will be interesting to know additional details of the redox process involving oxygen. The new edge path proposed for Mn^{4+} migration is a nice accomplishment that can be used for the design of high-capacity materials.

Reviewer 3:

The modeling work provided a coherent picture of how lithiation occurred in the Li_xMnO_3 phase, as part of the Li-excess cathode materials, the reviewer stated. The reviewer was left with two questions on the simulation results. The first referred to Slide 10, where the modeling work successfully explained the voltage difference between the first charge and discharge curves. However, the experimental work also showed large difference in the charge and discharge capacity. The reviewer asked can the modeling work shine some light on this issue. On Slide 9, oxygen evolution was predicted to occur when x was greater than one (Li_xMnO_3). However, based on the open-circuit voltage (OCV) comparison, it seemed to the reviewer that the discharge capacity was given by x greater than one, where x varies between two and one. The reviewer's question was whether this mean no oxygen vacancy will be generated during the activation process and can oxygen evolution be simulated along with the Li removal.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The project team has a number of collaborations with other modelers and researchers examining these complex materials, the reviewer noted.

Reviewer 2:

It seemed to the reviewer that collaborations with the Massachusetts Institute of Technology (MIT) and ANL teams are going very well.

Reviewer 3:

Excellent collaborations and synergies with other DOE laboratories and industry were noted by this 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 plans to wrap up studies on Li_2MnO_3 , the reviewer noted.

Reviewer 2:

Additional investigation of the oxygen participation in the redox process seems very important, as it is strongly related to the evolution of stable or unstable crystal facets as a function of O_2 from the surface, the reviewer stated.

Reviewer 3:

The reviewer repeated the earlier question of whether oxygen evolution can be simulated along with the Li removal.

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

Reviewer 1:

This project will lead to improved high-energy-density oxide electrode materials, which should reduce costs and enable further electrification of the nation's vehicles, resulting in improved gas mileage, the reviewer predicted.

Reviewer 2:

The project is shedding light on the stability and potential improvements that can be introduced into high-capacity cathode powders. That, the reviewer continued, is very related to petroleum displacement, as it will enable higher capacity batteries

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

Reviewer 1:

The PI has been very productive, the reviewer noted.

Reviewer 2:

Resources seem to be sufficient, the reviewer said, adding that based on the data and new information produced in this project, those resources seemed to have been well expended.

Studies on High-Capacity Cathodes for Advanced Lithium-Ion Systems: Jagjit Nanda (Oak Ridge National Laboratory) - es106

Presenter

Jagjit Nanda, Oak Ridge National Laboratory.

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:

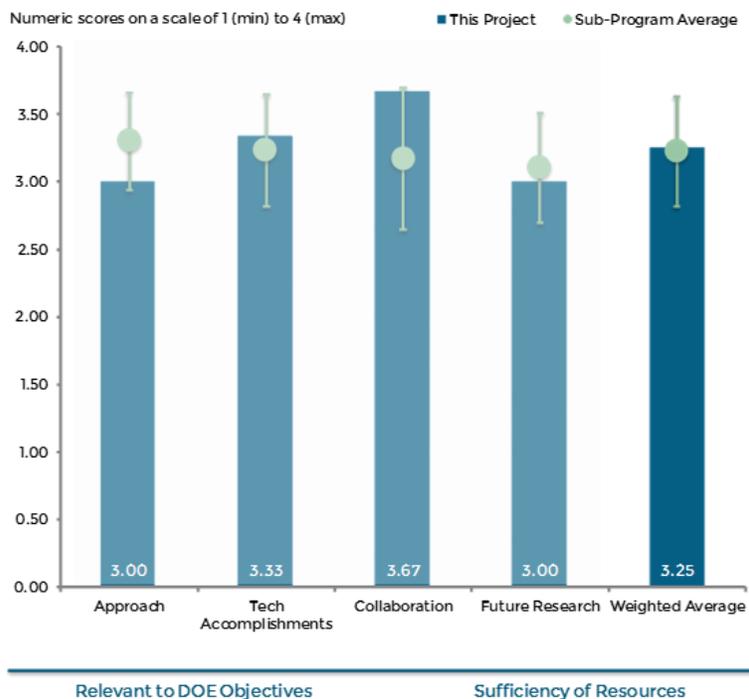
The project, in the reviewer's opinion, had two key tasks that were not necessarily interrelated, potentially resulting in the project's impact being diluted.

Reviewer 2:

The reviewer cited a two-fold projective objective, first, to understand the role of Li_2MnO_3 in the performance of LMR-LLC cathodes and correlate the bulk structural and interfacial changes in the Li_2MnO_3 component with its performance, and second, to develop alternate multivalent cathodes, $\text{Li}_2(\text{NiCu})\text{O}_2$ with high specific capacity. The reviewer noted that some time was also spent on the EIS behavior of the LMR-LLC cathodes, which the reviewer believed was not well connected with the objective of seeking structure versus performance correlation in the LMR-LLC cathodes. It is interesting to study Li_2MnO_3 alone during lithiation/delithiation cycling to understand its behavior in the composite cathode, the reviewer agreed, but found it unclear why this material was studied in the thin-film and slurry electrolyte electrode forms. The reviewer noted that, with the low specific discharge capacities, the extent of delithiation in Li_2MnO_3 is less than in the composite cathode. Overall, the reviewer said, the approach seems feasible and consistent with the program goals.

Reviewer 3:

$\text{Li}_2\text{Cu}_x\text{Ni}_{1-x}\text{O}_2$ is an interesting system, the reviewer said, and can be a candidate high-voltage and -capacity cathode material. However, the reviewer went on, initial capacity decay and oxygen evolution at less than 4.0 Volt (V) should be explained and the relationship between capacity decay and oxygen evolution should also be discussed.



es106

Figure 2-12 Studies on High-Capacity Cathodes for Advanced Lithium-Ion Systems: Jagjit Nanda (Oak Ridge National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer considered that the team did a good job in characterizing Li_2MnO_3 and LMR/NMC cathodes using a number of analytical tools such as EIS, Raman, and Xanes. These were done quite effectively, the results are of high quality and the authors reached careful conclusions in the reviewer's estimation. The reviewer termed the work with Li_2CuO_2 challenging but encouraging, adding that although the current data are far from promising (most of the capacity being at a low voltage), an opportunity to tailor the material in future studies has probably been opened.

Reviewer 2:

The reviewer said study $\text{Li}_2\text{Cu}_x\text{Ni}_{1-x}\text{O}_2$ cathode's electrochemical stability and capacity retention.

Reviewer 3:

The reviewer noted some interesting and useful observations on the delithiation behavior of Li_2MnO_3 . The formation of MnO_2 at high voltages is expected, the reviewer said, but asked if there was any gas (oxygen) evolution along with it at these high potentials (4.7 V). The reviewer was unclear as to why this material was studied in thin-film form as well as slurry electrode form. In either case, delithiation seems to be equally difficult, making it difficult to take cathode to deep delithiation. Likewise, the reviewer was unsure what to make of the EIS behavior, which is expected to be a function of voltage or degree of delithiation. The preliminary performance data on $\text{Li}_2\text{Cu}_x\text{Ni}_{1-x}\text{O}_2$ are encouraging, the reviewer said but there is still considerable oxygen evolution (favored thermodynamically) at these potentials. The reviewer saw no clear strategy presented on mitigating this oxygen evolution and wondered if cation substitution would alter the charge potential. The cyclic stability of $\text{Li}_2\text{Cu}_x\text{Ni}_{1-x}\text{O}_2$ has been improved, but the voltage profile is still not attractive, with low potentials for the second Li. Finally, the reviewer reiterated that overall progress is good and directed toward the DOE goals.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

An excellent collaborative team, the reviewer said.

Reviewer 2:

There are good ongoing collaborations with the other DOE laboratories and external university, and U.S. Department of Defense (DOD) collaborators, in the reviewer's opinion.

Reviewer 3:

The PI has developed collaborations with LBNL, Brookhaven National Laboratory, ANL, National Accelerator Lab and the Ford Motor Company, the reviewer observed.

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 is important to stabilize $\text{Li}_2\text{Cu}_x\text{Ni}_{1-x}\text{O}_2$ structure at high voltages, the reviewer said.

Reviewer 2:

The reviewer noted that the project is ending this year, with the focus on the high-capacity 2-Li copper (Cu)-Ni oxides, specifically to reduce particle size to improve kinetics, eliminate impurities and improve the stability through cation substitution. Finally, these cathodes will be studied to determine the stability of redox active Cu

and Ni using in situ synchrotron XAS and diffraction. These plans, the reviewer said, are consistent with overall goals of the Applied Battery Research (ABR) program.

Reviewer 3:

Noting that the project team now wants to work with this 2-e Li_2CuO_2 cathode, the reviewer suggested that the material be explored exhaustively without the distraction of other, ancillary projects. The PI, in the reviewer's estimation, is well experienced to explore its full potential. The reviewer, however, expressed a concern about this material, asking if there is any dissolution a la spinel and inquiring about its high-temperature behavior.

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

Reviewer 1:

The project does support DOE goals, the reviewer said, because high-voltage cathodes are critical for developing high-energy-density and lower-cost batteries.

Reviewer 2:

The reviewer noted that high specific energy, long cycle life and low cost are the performance drivers for Li-ion batteries in electric vehicles and that LMR-LLC cathode materials are promising due to their high capacities at high voltages, and possibly their low cost from the high Mn contents. However, their performance degradation upon cycling, both in capacity and voltage, are impediments to their use in Li-ion cells. This project, the reviewer observed, is aimed at understanding and mitigating these failure modes and is developing a high-capacity cathode, $\text{Li}_2(\text{CuNi})\text{O}_2$ for high-energy Li-ion cells.

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

Reviewer 1:

The funding level seems right, the reviewer said.

Reviewer 2:

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

PHEV and EV Battery Performance and Cost Assessment: Kevin Gallagher (Argonne National Laboratory) - es111

Presenter

Kevin Gallagher, Argonne National Laboratory.

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, the reviewer said, is a well-focused project to develop design and simulation capabilities for assessing performance and cost of Li-ion batteries.

Reviewer 2:

The reviewer praised this as a very dynamic effort to make BatPaC a useful tool and predicted that it will continue to be so for years as new designs and materials are identified. The BatPaC model development work contributes

greatly to the improvement in performance and cost prediction of known battery chemistries, the reviewer said, noting that it was clear a lot of work went into the development effort for modeling both cell and – to some degree – battery pack costs. The described change in approach, in the reviewer’s opinion, allows for improved results that fit actual vehicle usage. Finally, the reviewer remarked, a cost variable that should be added is that cell fabrication and pack build may be done in very different locations.

Reviewer 3:

The PI, the reviewer opined, knows the critical input needed for high reliability, cost and performance estimates.

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 towards DOE goals.

Reviewer 1:

BatPaC has been released and used widely by the battery community, the reviewer observed.

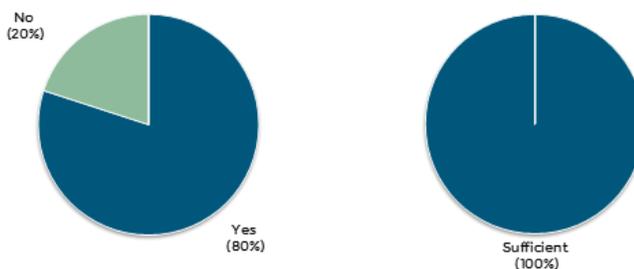
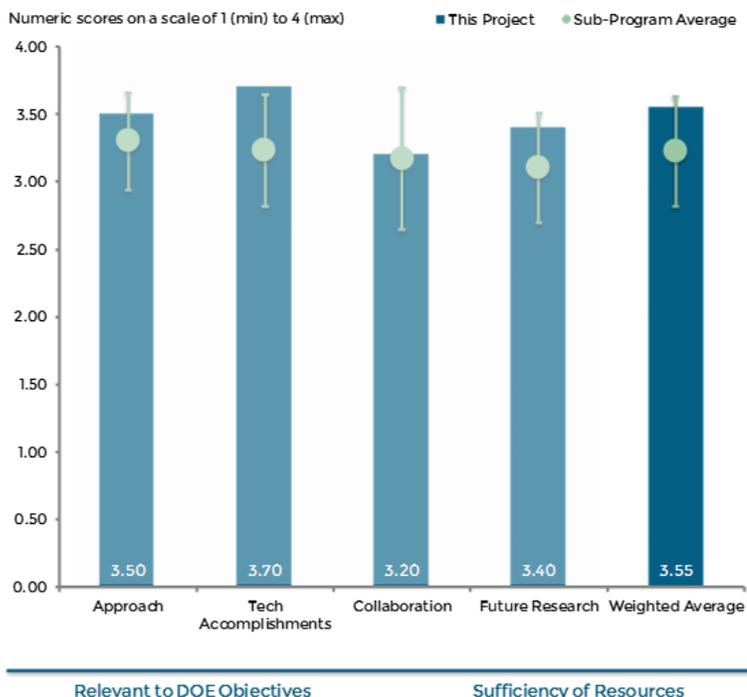


Figure 2-13 PHEV and EV Battery Performance and Cost Assessment: Kevin Gallagher (Argonne National Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The team has done an excellent job, the reviewer said, in providing guidance and recommendations for electrode loadings, thicknesses/transport limitations for EV targets, although the reviewer could not recall having seen the same calculations for PHEVs. This is very useful guidance for battery developers and highly relevant, the reviewer continued, but a high-level summary of assumptions, a short note on the models' limitation might be a very useful aid to better comprehension. The reviewer was left with several questions; first, was the charging situation considered in continuous power demand calculations, and if so, up to what rate levels. Second, how do the rapid gas discharge pathway calculations fit into this project. The reviewer noted that the assumptions for the Li/S model were missing – how much excess Li was there and what were the current collector assumptions.

Reviewer 3:

The technical accomplishments were clear in the tables presented, the reviewer noted, and the slide showing the value of the advanced cathode work and the potential cost and volume savings was very good. The significant role the anode plays in cost and volume savings was also informative and may, the reviewer speculated, drive more work on this system. The model provides directional cell development toward a Mn-rich cathode and Si/Gr composite anode as the likeliest cost winner. Additional benchmark test work will of course, identify if this is the best performance/cost winner.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Noting that collaboration partners included cell materials developers and manufacturers, as well as battery manufacturers, regulatory groups and one of the world's largest automotive battery users, the reviewer added that this type of collaboration is needed to develop and validate the system from both technical and business perspectives.

Reviewer 2:

The partners – battery developers and producers – will be able to validate the model, the reviewer observed.

Reviewer 3:

The reviewer suggested that collaboration with significant, high-volume cell manufacturers via confidential information exchange agreements to include more real-world information could be an improvement opportunity toward a greater level of reality in output. The reviewer also suggested that this might best be accomplished by an organization outside of ANL which can assure collaborators of information protection, while allowing ANL modelers access to genericized model data.

Reviewer 4:

While collaboration has been good, the reviewer said, there are more opportunities to expand.

Reviewer 5:

The reviewer noted there was no mention of involvement by electrode manufacturers.

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 highly relevant and useful, the reviewer said, especially electrode thickness calculations, updating of cost models, energy demand calculations and fast charging studies. Because virtually all suppliers are moving toward a single cathode system, the reviewer did not recommend the study be carried out unless it was desired to validate the model using the Volt as a test case.

Reviewer 2:

The presentation, the reviewer remarked, points to a critical role that the anode plays in the volume and cost, but this effort is not clearly included in the future work, unless the blended cathode was intended to be a blended Si/Gr anode. While acknowledging the need for fast charging to facilitate extended driving range, the reviewer called for more details on how the fast charging work will be included in the BatPaC future work to assess the value of its being called out as a focal point for future work.

Reviewer 3:

The future work is well defined and will add to the usefulness of the model, according to this reviewer.

Reviewer 4:

The reviewer expressed support for looking more at sulfur.

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

Reviewer 1:

This project fits well within the overall DOE program, the reviewer said, as having a reliable model for performance simulation and cost assessment is very useful for tracking progress as well as benchmarking and projecting various battery systems.

Reviewer 2:

The BacPaC model helps identify ways a cell manufacturer can realize a meaningful cell cost reduction, the reviewer noted, and because cell cost is at least 50% of an automotive battery cost, it represents one of the biggest hurdles for adoption of this technology as a viable alternative to the internal combustion engine (ICE). Consequently, any system that allows a meaningful cell cost reduction supports the DOE objective to reduce petroleum usage, the reviewer concluded.

Reviewer 3:

The model will lead to optimized decision making on designing and building batteries, the reviewer predicted.

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

Reviewer 1:

The resources provided should be sufficient to meet the stated milestones, in the reviewer's opinion.

Reviewer 2:

The ANL modelers and the industry support will be sufficient to achieve the milestones, the reviewer agreed.

Open Architecture Software for CAEBAT: John Turner (Oak Ridge National Laboratory) - es121

Presenter

John Turner, Oak Ridge National Laboratory.

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, addressed the barrier that there is no common framework for integrating battery modeling efforts and standards for battery modeling, and is well coordinated with other CAEBAT projects.

Reviewer 2:

Approach 1 is summarized schematically in Slide 6: CAEBAT [Computer-aided engineering of batteries] Open Architecture Software

Vision - a Virtual Test Bed, the reviewer noted, adding that it was unclear whether the validation piece falls under the scope of this project. Even if some of the contributions are from external sources (test results from ABR, Batteries for Advanced Transportation Technologies [BATT] and industry), the reviewer believed it would be useful to show more examples of various model outputs agreeing with experimentally generated data. Given the complexity of the work and the broad suite of integrated components, it is difficult to generate a very simple overall statement of objectives and work flow, the reviewer acknowledged, but this would be useful. Also, it was not entirely clear to the reviewer which, if any, of the modules were created under the program and which were merely integrated into the open architecture software (OAS). The decision to include four software suites (from various commercial partners) enhanced the flexibility and lowered overall risk, the reviewer concluded.

Reviewer 3:

The objective of this project was somewhat unclear to the reviewer. It was evident that this platform allows the combination of commercial and public software through a standard interface; however, the specific type of problem that motivates this synergy needed clarification, in the reviewer's opinion, or at least the provision of a matrix of the range of physical problems that may be addressed using this technology.

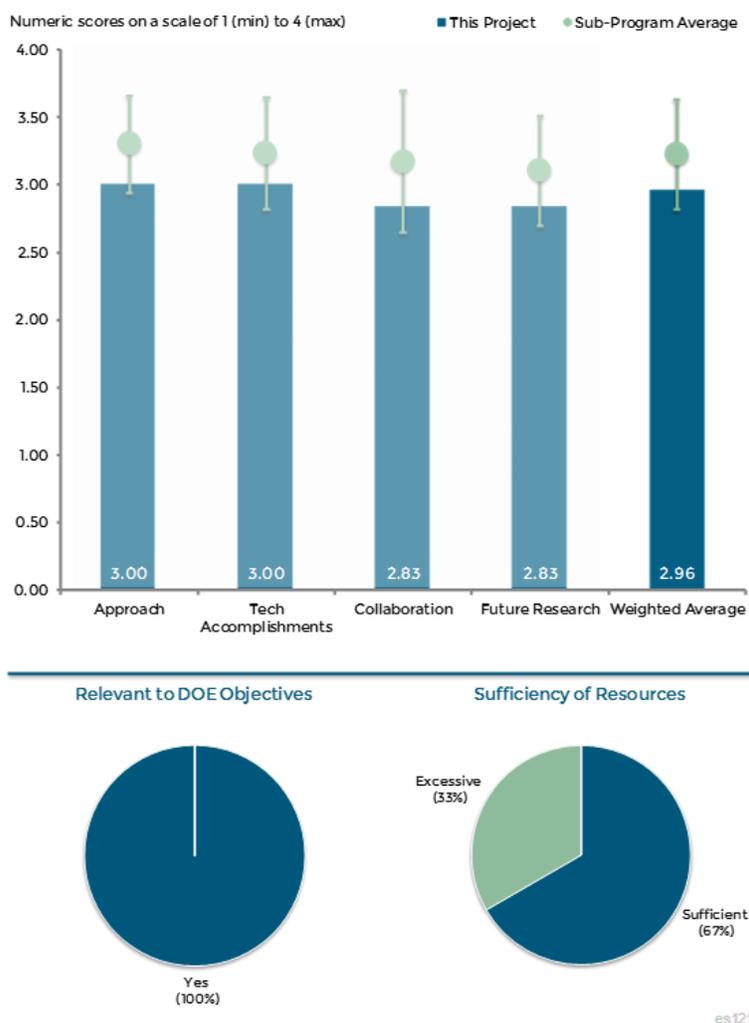


Figure 2-14 Open Architecture Software for CAEBAT: John Turner (Oak Ridge National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

To the reviewer, the ambitious technical goals appeared largely complete and that a notable endorsement of the value of the work was visible in the Virtual Integrated Battery Environment (VIBE) download statistics, illustrating the tool's significance to industry and academia. File-based coupling of electrochemistry, transport, and electrical and mechanical stress models extends the usefulness to many very relevant problems such as thermal management and internal short response prediction, and the flexibility to accommodate various form factors and array configurations is also useful and essential, in the reviewer's estimation.

Reviewer 2:

It was unclear to this reviewer how the types of example problems being solved are distinguished from those that can be solved with existing commercial, multiphysics software (e.g., COMSOL). The reviewer inquired about the capability that is being added here, and the impact, with this platform that exceeds what is commercially available. A clearer benchmark of existing commercial platforms and deficiencies would better support the research.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Extensive coordination and collaboration efforts were critical to success for this work, given its integrative nature, and the diversity of the participants – academia, industry and other DOE partners – was clearly shown, the reviewer said. The reviewer observed that the multi-faceted engagement efforts and the significant publications and presentations on the subject were likely helpful in giving the work some visibility, as illustrated by the many users. It was also clear to the reviewer that there is a structured approach to getting and incorporating feedback from initial users at every level (including creation of users' mailing list), and that the intent is to continue incorporating revisions based on community feedback. The reviewer asked if there is a central introductory overview online designed to communicate the scope of the capabilities and vision written not for the end-user, but for the researcher and industry member who would have a use for the results. This might accelerate dissemination, in the reviewer's view.

Reviewer 2:

The reviewer would like to know what the role is of the GM-ANSYS and CD-Adapco teams in this project and how these teams have been integrated into the research effort.

Reviewer 3:

The reviewer recommended that the project team double check to see if all the models developed in other CAEBAT projects are compatible with VIBE/OAS.

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 work is largely complete, the reviewer noted, but in the longer term, adding new features does not provide a lot of information. Elaboration in this area would be useful to understand which technical areas will be pursued next. It would also be useful to better understand the comment (Slide 24) "compatible with at least some components of CAEBAT." The reviewer asked which components and what is the reason for the incompatibility of others. The reviewer wondered if this is a problem to be solved or is it of little importance.

Reviewer 2:

The PIs should clarify the advantages of this platform per the comments in the Technical Accomplishments and Progress section, the reviewer said.

Reviewer 3:

The reviewer wondered if OAS can interact with LS-Dyna and Fluent-API.

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

Reviewer 1:

Validated and reliable models are invaluable in accelerating development and shortening time to market through efficient and less costly optimization, the reviewer pointed out. Thus, having an OAS tool available not only to industry, which may have similar tools in some cases, but for the smaller and growing entities which may have great ideas but rely heavily on modeling, will encourage innovation and growth.

Reviewer 2:

This project is focused on advanced simulation tools for electrified vehicles, which is a key enabling technology for petroleum displacement, the reviewer said.

Reviewer 3:

The reviewer considered that this is an integral part of developing software tools to design and model batteries.

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

Reviewer 1:

Given the technical complexity, the multi-partner, multi-platform approach, the resources did not seem excessive to this reviewer, who also noted that tremendous resources are required for broad-suite, comprehensive testing, so if this tool can allow test matrices to be reduced, its value will be well justified.

Reviewer 2:

These resources may be excessive if the impact of the research is not more clearly defined, the reviewer said.

Composite Electrolytes to Stabilize Metallic Lithium Anodes: Nancy Dudney (Oak Ridge National Laboratory) - es182

Presenter

Nancy Dudney, Oak Ridge National Laboratory.

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:

Noting that one of the main approaches, namely, “use theory and simulation to explore mechanical stability” has apparently been postponed because of the variability in the measured ionic conductivity caused by the presence of impurities, the reviewer remarked that it may be helpful to know whether these impurities would also cause problems with mechanical properties, and thus provide deeper insights into the role of impurities at interfaces.

Reviewer 2:

The promise of a solid electrolyte for Li batteries is high, the reviewer said, and the initial technical approach was interesting, but this technical plan, in the reviewer’s opinion, got waylaid. Because it has always been understood that processing and manufacturing would be among the larger issues, the reviewer found it unsurprising that this has been the sticking point in this research. However, the shift in focus appeared to the reviewer to be quite academic. It is important to keep in mind, the reviewer asserted, that the intention has always been to scale this up for manufacturing. Exposure is quite a nebulous term, especially on a high-speed manufacturing line; the impact of exposure time was never discussed, the reviewer said, and is likely to be the key point in commercialization. Additionally, it needs to be clear that the liquid electrolyte is not adversely impacting SEI formation. A clear focus must be maintained on the commercial applicability and reproducibility of this environment to ensure that this research has its intended impact, the reviewer concluded.

Reviewer 3:

Noting excellent attention to detail and extra steps taken to separate differences in experimental set-ups, the reviewer offered that it might be very beneficial to establish a baseline and the SOP to detect and characterize the outlier results more rapidly; this in turn might open an opportunity for the new inventions.

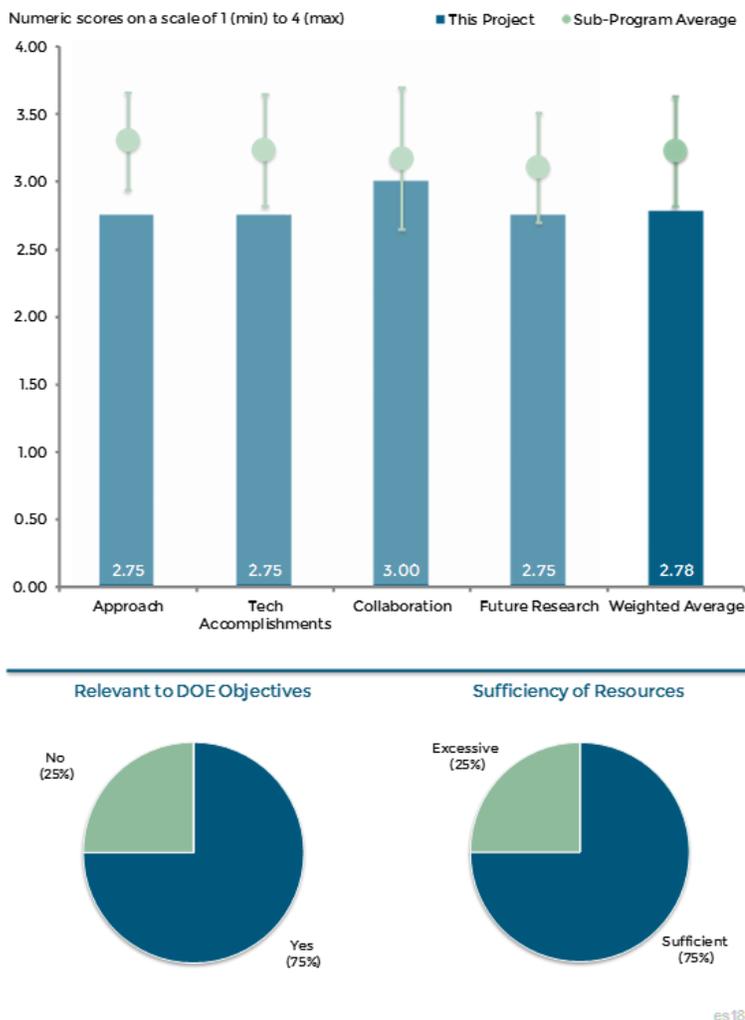


Figure 2-15 Composite Electrolytes to Stabilize Metallic Lithium Anodes: Nancy Dudney (Oak Ridge National Laboratory) - Electrochemical Energy Storage

Reviewer 4:

The reviewer concluded that this project appeared to be a mess of uncontrolled process variations. While some of the outcomes may be of interest, it seems that it would be necessary to get to a baseline performance level where the variation is removed is necessary in order to proceed with the introduction of controlled variations.

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 towards DOE goals.

Reviewer 1:

It may be helpful, the reviewer suggested, to use depth profiling techniques (e.g., XPS, Auger, SIMS, Rutherford Backscattering, Elastic Recoil analysis) to determine the species present at the interface between polymer- and ceramic-electrolyte interfaces to resolve the observation that “subtle differences in composite processing have large impacts on the bulk conductivity.” These depth profiling techniques have been used successfully in the development of doping of the p-n junctions in the microelectronics industry, the reviewer added. It may also be helpful to measure ionic conductivity across the layered polymer-ceramic electrolyte interface as a function of applied stress to help understand whether interface contact area plays a role (e.g., contact area at the interface increases with increasing normal load).

Reviewer 2:

The reviewer said introduction of the statistical tools and standards might further accelerate the progress.

Reviewer 3:

To this point, the work does not appear to be reproducible in another lab or even after the glove box was changed for maintenance, the reviewer observed, adding that it is important to know to what degree the environment is saturated. While this study is interesting, the reviewer went on, it still appears the Ohara ceramic is the best. While this may be true for bulk conductivity, the effective conductivity including the interface may be limiting. The reviewer proposed that it might be best to showcase the improvement this research is providing to show progress toward the original technical goals and it needs to be clearer to what degree. A fair bit of this work seemed to the reviewer to be better suited to the DOE Office of Basic Energy Sciences (BES) as opposed to VTO. The reviewer stressed that greater focus should be applied to understanding the interface.

Reviewer 4:

The reviewer believed this project possibly needs to start from zero.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer was pleased to note not only outstanding collaboration efforts, but coordination of the materials studied.

Reviewer 2:

Noting an appropriate collaboration of ceramic electrolyte partners, the reviewer believed that engagement of a commercialization partner would help make this research more readily applicable to the industrial process.

Reviewer 3:

The reviewer was not quite able to determine where collaborators are contributing.

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 research project is very challenging, the reviewer assessed, but the PI understands the critical issues and has a well-thought-out plan to attack them.

Reviewer 2:

The reviewer suggested it may be helpful to use depth profiling techniques (e.g., XPS, Auger, SIMS, Rutherford Backscattering, Elastic Recoil analysis) to determine the species present at the interface between polymer- and ceramic-electrolyte interfaces to resolve the observation that “subtle differences in composite processing have large impacts on the bulk conductivity.” These depth profiling techniques have been used successfully in the development of doping of the p-n junctions in the microelectronics industry, the reviewer added. It may also be helpful to measure ionic conductivity across the layered polymer-ceramic electrolyte interface as a function of applied stress to help understand whether interface contact area plays a role (e.g., contact area at the interface increases with increasing normal load). The reviewer also suggested that it may be helpful to predict theoretically what species present at the interface would be helpful to ionic transport.

Reviewer 3:

The reviewer termed the Proposed Future Work section sparse, saying it would be best to refocus the last year of this project to reflect some of the critiques of the work.

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

Reviewer 1:

The development of higher energy-density, longer cycle-life batteries with improved safety profiles would accelerate the electrification of the transportation sector, the reviewer predicted.

Reviewer 2:

The success of this project will enable battery systems that can address DOE performance and cost targets, the reviewer said.

Reviewer 3:

Even were this a feasible, well-performing program, the reviewer said, adding that it currently is not, the approach is questionable. The reviewer expressed remaining concerns about the viability of solid Li in a large-format cell that might be subjected to a physical breach by outside forces. The reviewer clarified that expression of this concern was not to suggest that the performance of the solid Li system is unattractive or even unattainable, merely that the reviewer worried about whether it can ever truly be safe from external issues.

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

Reviewer 1:

An excellent team and access to the characterization tools, was the reviewer’s comment.

Reviewer 2:

The reviewer noted that the budget presented was for FY 2013 and FY 2014. The reviewer further asserted that no comment can be made, as this appears to be sloppy preparation.

In-Situ Solvothermal Synthesis of Novel High-Capacity Cathodes: Feng Wang (Brookhaven National Laboratory) - es183

Presenter

Feng Wang, Brookhaven National Laboratory.

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:

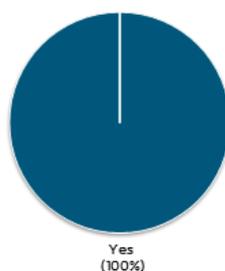
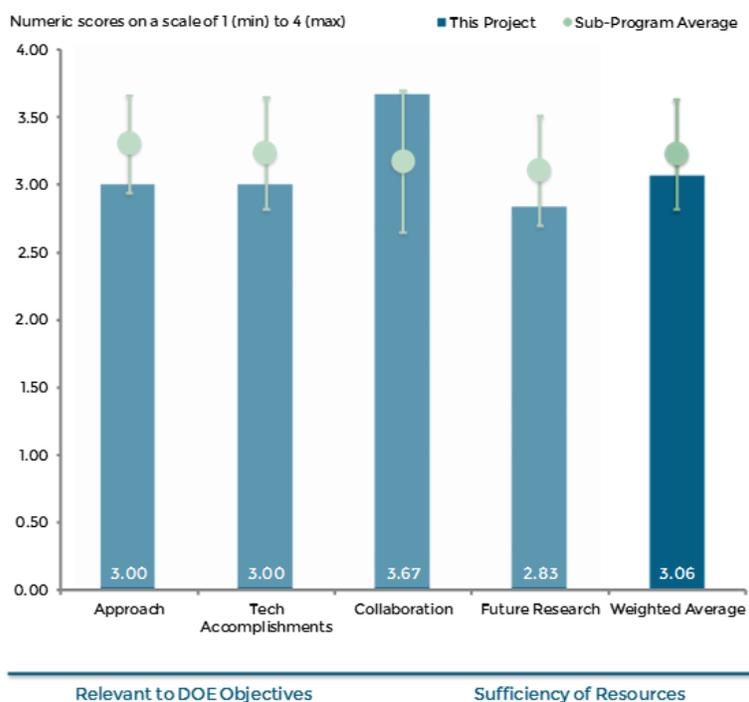
Describing the objective as being to investigate thermodynamic and growth kinetics using various in-situ methods, the reviewer predicted that in-situ study of batteries will significantly and directly help to understand the structure and different phases/compositions.

Reviewer 2:

The reviewer described the project objective as being to develop high-capacity cathodes, including polyanionic cathodes (LiVPO₄X) with multi-valent redox capability for high capacity, with high voltage (PO₄) and open framework for high Li⁺ mobility. Also, a small effort is placed on Cu-V-oxygen (O) and Cu-Fe-fluorine (F) cathodes of high capacity. For a proper assessment of the new materials, the reviewer cautioned, it is important that the synthesis method results in phase-pure materials and allows good control of stoichiometry and morphology. The approach is based on utilizing the in-situ solvo-thermal synthesis developed in this project which 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. The technique appears to be quite useful in the development of new materials, the reviewer eventually observed. Three different families of cathode were explored; some of them displayed high capacities, but only at low potentials. The result, the reviewer concluded, is that there is not much improvement in the energy densities compared to the conventional cathode materials.

Reviewer 3:

Aside from the in-situ work in reactors, the reviewer said, the other topics are either low-impact or variations of work previously out. The reviewer did not consider it a negative, but also noted some overlap with work done under project es051.



es183

Figure 2-16 In-Situ Solvothermal Synthesis of Novel High-Capacity Cathodes: Feng Wang (Brookhaven National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

Good progress has been made, the reviewer noted, toward developing the solvo-thermal and ion exchange syntheses processes for three different cathodes with in-situ determination of phase purity and composition, to wit, $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ nanocrystals of high power density, $\text{Li}(\text{Na})\text{PO}_5\text{F}$ with high Li content and Cu-V-O and CuFeF_2 cathodes of high capacity. The method appears to be quite useful to explore new cathode materials, in the reviewer's estimation. Of the three cathode materials studied, both $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ and $\text{Li}_x\text{Na}_{1.5-x}\text{VPO}_5\text{F}_{0.5}$ have low specific capacities, while the copper vanadates and fluorites have lower discharge voltages to make them appealing for the high-energy Li-ion cells. Overall, these studies are interesting from an academic perspective, the reviewer believed, but do not add much value from the application perspective. The reviewer recommended focusing more on materials that can offer improved energy densities compared to the conventional cathodes to take advantage of this method and to make these studies relevant to VTO.

Reviewer 2:

The team's work on micro-reactors and in-situ monitoring of reaction pathways is certainly very interesting and useful and the team has done a good job in characterizing the materials in the course of synthesis, the reviewer stated, expressing the belief that this was the strength of the work. The reviewer was left with one question, however, namely, how have these studies helped the authors redesign their synthetic procedures. Other aspects of the work, however, such as ion-exchange, lithium iron phosphate (LFP), Cu-V-O or Cu-Fe-F are low-impact studies, the reviewer said, the first being impractical, the second mature and the third offering too little capacity at high voltage.

Reviewer 3:

Both vanadate and fluorite compounds have such low potentials that they are not practically useful, in the reviewer's opinion.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted collaboration with a lot of relevant laboratories.

Reviewer 2:

This is a good collaborative project, the reviewer said, involving interactions with several laboratories and universities.

Reviewer 3:

PI has developed collaborations with many researchers at a number of national laboratories and universities, the reviewer observed.

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 is unsure which new high-capacity Ni-Mn cathodes the authors are planning to synthesize. The reviewer believed that if the authors leverage the techniques they have developed so far then there is certainly a lot of good value in the future work. On the polyanionic front, the reviewer recommended that the various researchers reach some type of understanding to prevent overlap. This reviewer said that fluorites and vanadates have low capacity at high voltages and expressed doubt that it is worthwhile pursuing them.

Reviewer 2:

The future plans are to continue development of polyanionic cathodes, (Li(Na)VPO₅F_x), to explore polyanion-type ternary and quaternary Li-V phosphate cathodes, i.e., Li-V-PO₄ cathodes, to investigate the new α -CuVO cathodes further and to develop new, high-capacity Ni-Mn-based oxide cathode (both layered and spinel). The solvo-thermal synthesis with in-situ analysis to ensure phase purity and composition enables such exploratory work and the reviewer urged this project continue to identify and screen new cathode materials that have the potential to provide higher specific energies compared to state-of-the-art cathode materials.

Reviewer 3:

It is proposed to apply existing in-situ methods to different cathode materials, the reviewer observed, adding that this is not much different from previous work.

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

Reviewer 1:

The work is certainly relevant, the reviewer stated, especially the reactor work/in-situ monitoring studies, which are insightful and instructive.

Reviewer 2:

Low specific energies and high costs are the limitations of current Li-ion batteries for EV applications. While several engineering improvements have contributed to a marginal increase in specific energy recently, the reviewer noted, new, high-specific-energy materials are desired to fill the gap. State-of-the-art cathode materials provide capacities of only about 160 mAh/g, about half of capacities possible from C anodes. The present project, the reviewer concluded, is aimed at developing new cathode materials with much higher specific capacity/energy.

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 for the scope of the project, according to this reviewer.

Lithium Bearing Mixed Polyanion Glasses as Cathode Materials: Andrew Kercher (Oak Ridge National Laboratory) - es184

Presenter

Nancy Dudney, Oak Ridge National Laboratory.

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:

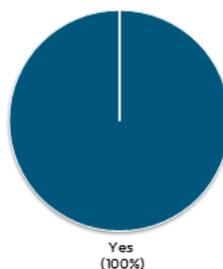
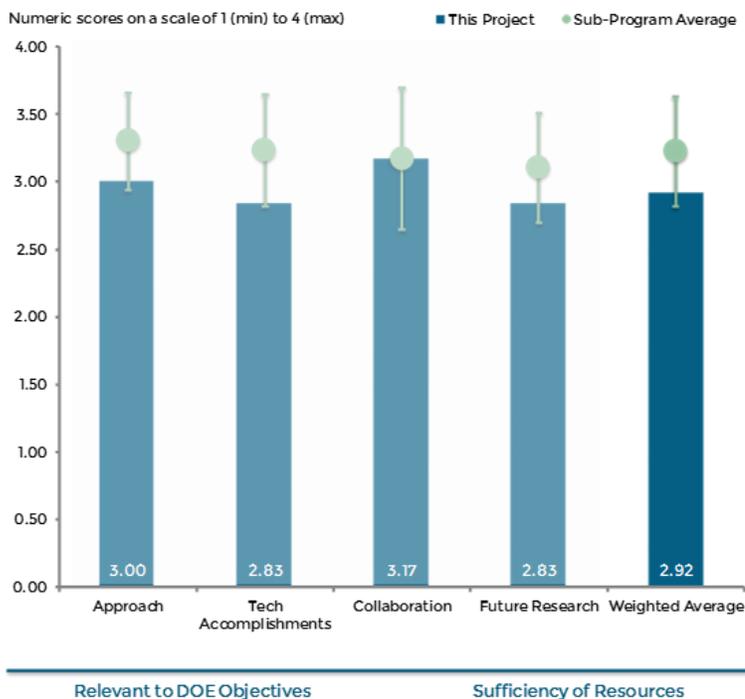
Polyanion substitution increased the specific capacity and electronic conductivity, the reviewer observed.

Reviewer 2:

This was a high-risk, high-payoff project, the reviewer stated, noting that the project team had tried various avenues to improve upon several intrinsic limitations of glassy materials for use as high-energy electrode materials.

Reviewer 3:

The premise for this project is that the mixed polyanion glasses may alleviate the problems of poor conductivity and irreversible phase transitions posed by traditional crystalline polyanion cathodes of theoretically high capacities, the reviewer stated, offering the examples of LiMnBO_3 , LiCoBO_3 and $\text{Li}_2\text{CoSiO}_4$. The objective of the work, the reviewer went on, is to synthesize and mix polyanion glasses in the phosphate family containing a variety of transition metal cations to have specific energies exceeding that of LiFePO_4 , specifically V-substituted Fe phosphate glasses such as $\text{Fe}_4(\text{P}_2\text{O}_7)_3$ with 30-50% vanadate, which showed improved specific capacity and rate performance. To achieve high capacities, the reviewer said, conversion reactions may be used in lieu of or in addition to insertion reactions. However, conversion reactions in crystalline form have considerable hysteresis and poor reversibility. In glassy form however, the conversion reactions (charge) may be easier (for recharge), in principle. High capacities have been achieved with some of the mixed polyanions glasses as expected, but the capacity fade is still high. Nonetheless, the reviewer concluded, the approach looks promising and the project is well integrated with the other materials-based efforts.



es184

Figure 2-17 Lithium Bearing Mixed Polyanion Glasses as Cathode Materials: Andrew Kercher (Oak Ridge National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

Reasonably good progress, in the reviewer's estimation, has been made in synthesizing and evaluating the V-substituted, Fe-phosphate cathodes in glass state. High capacities have been realized with Fe-pyrophosphate and in Cu or Co meta-phosphate glass with 50% vanadate substitution. However, fade rate during cycling is rather high, especially with the conversion reactions. Moreover, the potentials for the second reaction are rather low, but may possibly be improved with suitable substitutions/dopants. A good comparison, in the reviewer's view, will be the specific energy of the cathodes, rather than their specific capacities. It was also shown that the phosphate glasses with vanadate or molybdate have similar total specific capacity and cycle performance and molybdate will avoid the environmental concerns with V. Overall, the mixed polyanion approach looks appealing, the reviewer said, but the benefits from these mixed polyanion glass compounds are not yet significant compared to the crystalline analogs or other cathode options being explored under VTO.

Reviewer 2:

The reviewer noted that the authors have developed several new compounds that clearly do not exhibit any potential for use as high-energy cathodes because discharge voltages are mostly below 2 V. In fact, the reviewer said, they have features similar to those of anodes and also undergo rapid fade.

Reviewer 3:

For the developed glass cathode, most capacity was contributed at voltages less than 2.0 V, a level not practically useful, in the opinion of this reviewer.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

There are good ongoing collaborations with MIT and Northwestern University on the XANES characterization and modeling of these cathode materials, respectively, said the reviewer.

Reviewer 2:

Collaborations have been developed with Brookhaven National Laboratory and MIT, the reviewer noted.

Reviewer 3:

The reviewer would have welcomed more collaborative work, especially from the characterization point of view.

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 research, the reviewer summarized, is to focus on the mixed polyanion glass cathodes with emphasis on increasing the free volume and conductivity for the multi-valent insertion reactions and improve the capacity fade, discharge voltage and the hysteresis for the conversion reactions. Also, the future plans are to extend these studies to non-phosphate and non-traditional glasses. Overall, these proposed studies are logical and provide alternate development pathways for the development of high-energy cathode materials to mitigate the performance limitations observed in the crystalline materials, in the reviewer's opinion.

Reviewer 2:

The reviewer was unsure any of the future tasks proposed will lead to any result substantially better than has been observed thus far. It may be, the reviewer speculated, that use of non-traditional glass-formers, of which

the reviewer wished the team had given some examples, might suggest a different direction to the investigation, because none of the traditional glass-formers yielded any interesting results. The reviewer raised a question concerning the effect of nanoparticles. Given the low probability of success with these materials, the reviewer wondered whether the project team might rethink its future plans and develop an aggressive, out-of-the-box idea for the remainder of the program.

Reviewer 3:

The reviewer cited a lack of strategy for improving cathode voltage and conductivity

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

Reviewer 1:

It is a high-risk project that, if successful, might be relevant, the reviewer thought.

Reviewer 2:

The limited range and high cost of Li-ion batteries are serious impediments to 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 and reduced overall battery cost. State-of-the-art cathode materials provide capacities of only around 160 mAh/g, about half the capacities possible from the C anodes. Thus, the reviewer concluded, there is a need to develop new cathode materials of higher specific capacities, possibly with multi-electron redox processes, as is being addressed in this project.

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

Reviewer 1:

Funding level seems right, the reviewer said.

Reviewer 2:

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

Significant Enhancement of Computational Efficiency in Nonlinear Multiscale Battery Model for Computer-Aided Engineering: Gi-Heon Kim (National Renewable Energy Laboratory) - es197

Presenter

Gi-Heon Kim, National Renewable Energy Laboratory.

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 an excellent project, the reviewer stated, addressing computational efficiency issues experienced in CAEBAT.

Reviewer 2:
The reviewer termed this a complex task that the team had approached with a focus on imparting maximum relevance to industry and general users and noted the segregation by time-scale as representing an elegant approach, with the great increase in computational speed providing evidence of the effectiveness of the strategy taken. Equally impressive to the reviewer was the fact that the increased speed came with no significant reduction in the accuracy and integrity of the results versus those achievable with much greater computing time.

Reviewer 3:
The project targets and approach appeared to the reviewer to be relatively clear.

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 towards DOE goals.

Reviewer 1:
Noting the target of achieving a 100 times faster computational speed had been defined and attained, and in some scenarios exceeded, the reviewer stated that this greatly enhanced the usefulness of the GH-MSMD. Code implementation in C++ and MATLAB, the reviewer continued, further strengthens the tool applicability. Integrating of the National Renewable Energy Laboratory’s (NREL) custom electrode domain model (EDM)

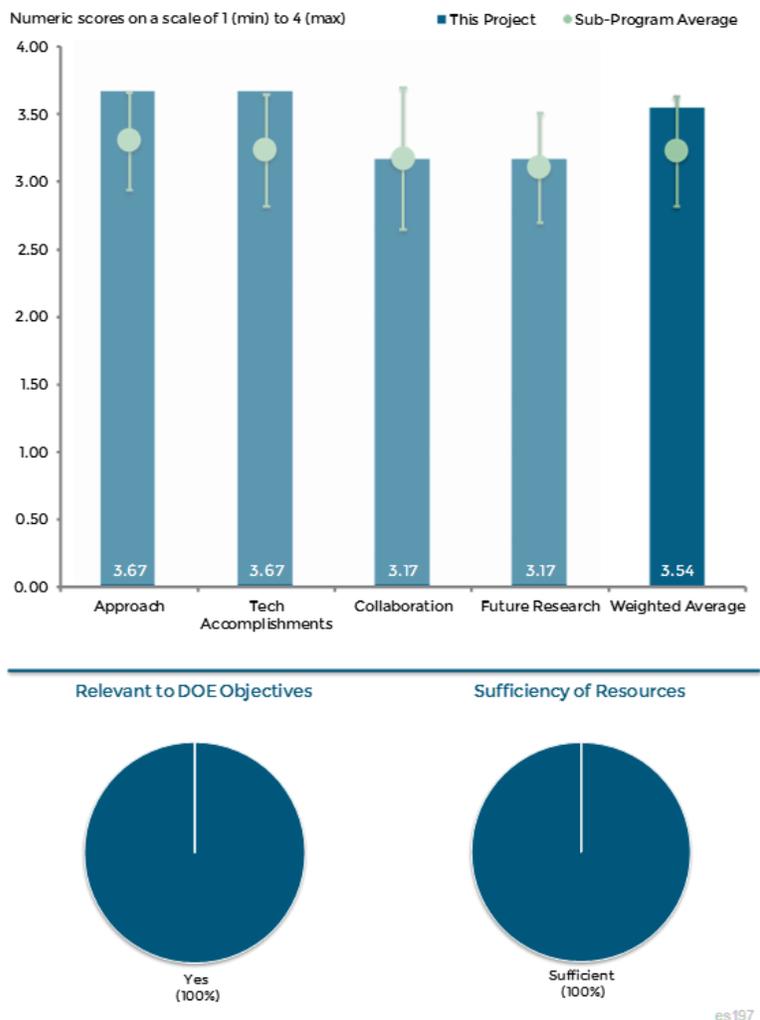


Figure 2-18 Significant Enhancement of Computational Efficiency in Nonlinear Multiscale Battery Model for Computer-Aided Engineering: Gi-Heon Kim (National Renewable Energy Laboratory) - Electrochemical Energy Storage

modules for electrochemistry, abuse reaction kinetics and ISC into ANSYS Fluent is a significant accomplishment, in the reviewer's estimation. The reviewer believed there is a significant opportunity to leverage partners from industry, ANSYS and other national laboratories with fabrication capability to conduct more validation work to address the challenging topics of ISC, fast charge, etc.

Reviewer 2:

To the reviewer, it appeared that the investigators had met their target in terms of the speed-up of the simulation process. One moderate concern the reviewer expressed concerned the generality of the method and how well it may be practically adopted in industry.

Reviewer 3:

The reviewer wondered if this model had been verified in OAS developed by ORNL.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The change in course from a direct University Partner (UP) to the UP working through ANSYS was not a negative one, in the reviewer's opinion, and possibly conferred some advantages. It was not clear to the reviewer what the status and plans for incorporation into ANSYS CAEBAT framework and ORNL OAS were. This, the reviewer said, was listed in 2014 as future work but was not shown this year under future work. The reviewer believed it would be helpful to understand where this fits in the larger scheme of things, as there are areas of overlapping research within DOE, some of which are certainly intentional.

Reviewer 2:

It seemed to this reviewer that the collaborative aspect of the research is moving forward with ANSYS. The reviewer expressed the hope that this will address the earlier comment made in the Technical Accomplishments and Progress section.

Reviewer 3:

The reviewer expressed a desire to see collaborations with vehicle and/or battery original equipment manufacturers (OEMs) on the pack-level model efficiency improvement.

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:

Extension of the time domain approach to development of a frequency domain GH-MSMD counterpart will be a challenging undertaking, but if successful will further broaden the applicability of the model to a more diverse range of engineering problems.

GH-MSMD is not intuitively understandable (unlike the original MSMD), but NREL is cognizant of this and is actively seeking to summarize, publicize and disseminate the features of the tool to encourage broad interest and usage.

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

Reviewer 1:

The reviewer described practical and commercially available tools for advanced simulation of battery technologies as key enablers for future, more-electrified vehicles.

Reviewer 2:

This tool promised to be an elegant and user-friendly tool that will have broad use in industry and academia to advance challenging engineering problems in a diverse range of areas, the reviewer predicted, and its contribution to optimized material, electrode, cell and pack design may help bring down the cost of battery technology. The tool will particularly benefit those users without their own capability in this area, the reviewer added. The ability to address problems spanning multiple engineering domains (fault evolution, thermal management, aging, etc.) is valuable, the reviewer stated, and the availability of a fast and robust tool can further support screening and assessment of new materials and battery designs.

Reviewer 3:

This project targets the computational efficiency improvement to promote CAEBAT employment, 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 are suitable for the project scope, the reviewer reiterated, while encouraging greater leverage of DOE partners for more hardware validation.

Mechanistic Modeling Framework for Predicting Extreme Battery Response: Coupled Hierarchical Models for Thermal, Mechanical, Electrical and (Electro)Chemical Processes: Harry Moffat (Sandia National Laboratories) - es198

Presenter

Harry Moffat, Sandia National Laboratories.

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 strategy of integrating C++ open-source framework (with its multi-physics models) into ORNL CAEBAT open architecture is worthwhile and of value, the reviewer stated, as the project undertakes to advance the sophistication of modeling's use in particularly complex aspects of various abuse conditions, such as the role of interfaces and surface phases, cell pressurization, porosity changes and geometrical complexity of the cell microstructure. To assist with tackling this challenging array of problems, the reviewer observed, the project leverages expertise from a diverse team of collaborators: Sandia National Laboratories (SNL), ORNL, Colorado School of Mines, Duracell and other groups, and is also facilitated by an open source github site.

Reviewer 2:

The approach seemed appropriate to the reviewer, in view of the final goal being an open source platform.

Reviewer 3:

The modeling effort is capable of predicting the battery effects of several abuse conditions, something that is needed in the vehicle and battery industries for battery design, the reviewer said.

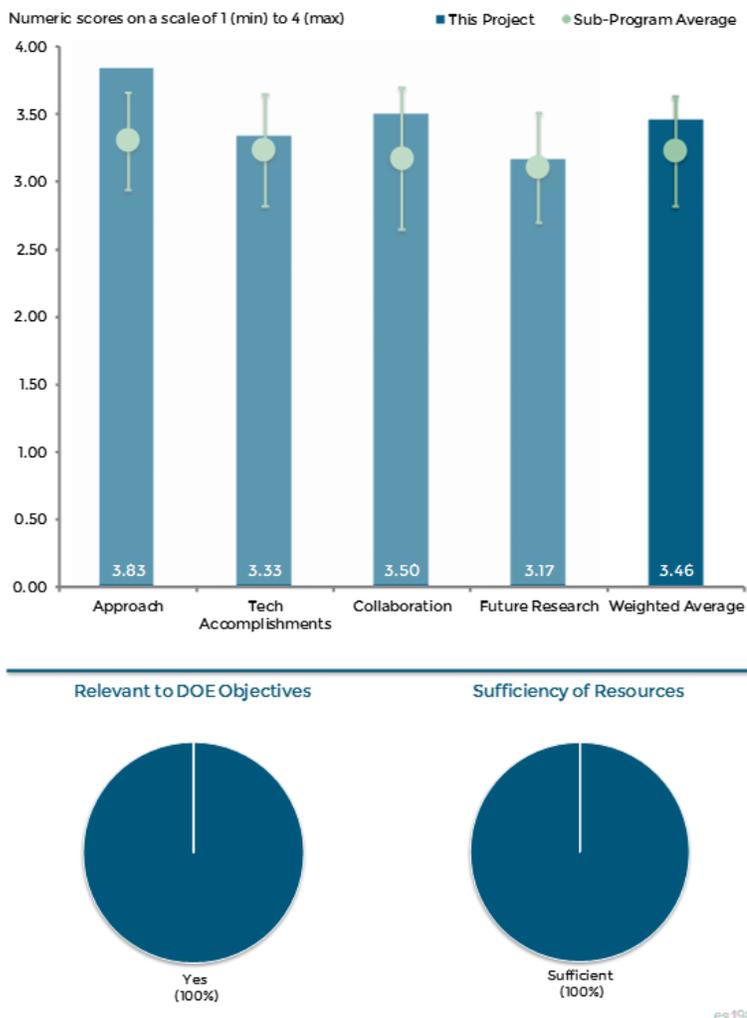


Figure 2-19 Mechanistic Modeling Framework for Predicting Extreme Battery Response: Coupled Hierarchical Models for Thermal, Mechanical, Electrical and (Electro)Chemical Processes: Harry Moffat (Sandia National Laboratories) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

It appeared to the reviewer that the technical accomplishments are generally on track.

Reviewer 2:

The project team has introduced an open-source multi-physics battery simulator ([cantrilbat.github.com](https://github.com/cantrilbat)) for mechanism development, and integrated the model into the CAEBAT architecture, duplicating existing capability with Cantera/1D electrode with added functionality (e.g., new transport coefficient algorithms for organic solvent salts), satisfying the go/no go gate. The reviewer summarized that Total Enthalpy Formulation introduces the capability of handling multiple phases and multi-physics terms (e.g., solid mechanics, partial saturation) that have previously been unavailable to the battery community. The result is a model offering numerous advantages over spherical models. The reviewer was left with several questions, however, including that of which chemistries have already been incorporated and which ones (thermodynamic, transport and kinetic data, etc.) are still needed. The reviewer asked is there an understanding of the computational power and processing time required for full solutions.

Reviewer 3:

The reviewer believed it was unclear if the models developed can be generic enough for both new and aged batteries and noted that the April 1, 2015 milestones seemed to have been delayed.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Noting excellent collaboration, with a framework for soliciting more collaboration through github, the reviewer expressed the view that adding another partner with recognized experience in Li-ion mainstream battery development and production would strengthen the list further.

Reviewer 2:

The reviewer found that the role of each collaborator was 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:

While deeming future objectives useful and valuable, the reviewer cautioned that they will certainly be extremely challenging. The reviewer expressed the hope that the processing power will be adequate to handle the increasingly complex model components and the desire for more details about plans for experimental validation with hardware.

Reviewer 2:

As a research code, this platform may be very effective, the reviewer said, but from a more applied perspective, the impact of this project may be somewhat limited.

Reviewer 3:

The reviewer wondered if the project could leverage other CAEBAT projects to reduce the time and efforts.

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

Reviewer 1:

This project, the reviewer said, takes the advanced state of models in this space and pushes them forward by addressing non-idealities that previous work has ignored through simplification. Adding another degree of fidelity to predict behavior under abuse conditions, once suitably validated, is an important contribution, the reviewer added, allowing much more complete and multi-parameter study than limited hardware testing where only a partial set of abuse conditions can be explored.

Reviewer 2:

Advanced simulation tools for greater insight into the safety and reliability of electrified vehicle system components represent a key enabling technology, in the reviewer's opinion.

Reviewer 3:

This effort will develop modeling tools to predict battery performance and thermal runaway, 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 are commensurate with the scope of work being addressed, in the reviewer's estimation.

Reviewer 2:

There are sufficient resources to achieve the proposed goals as planned, the reviewer stated.

Coupling Mechanical with Electrochemical-Thermal Models Batteries under Abuse: Ahmad Pesaran (National Renewable Energy Laboratory) - es199

Presenter

Ahmad Pesaran, National Renewable Energy Laboratory.

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 project objectives are well defined, and their linkage to the EV Everywhere Grand Challenge was described better than in any other poster the reviewer saw. The milestones were also well defined.

Reviewer 2:

To the reviewer, the coupled simulation approach seemed very good and the combination with experimental validation excellent. The reviewer recommended that early consideration be given the approach to the simulation/experimental cross-validation now to avoid excessive iteration between modeling and testing.

Reviewer 3:

The project is well designed, the reviewer said, and it addresses abuse conditions that could be experienced in PHEV 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 towards DOE goals.

Reviewer 1:

The numerical and experimental results, the reviewer said, are very good.

Reviewer 2:

The reviewer described the technical achievement to date as good and suggested that recruiting a battery company to collaborate in achieving the model’s validation on time might be advisable.

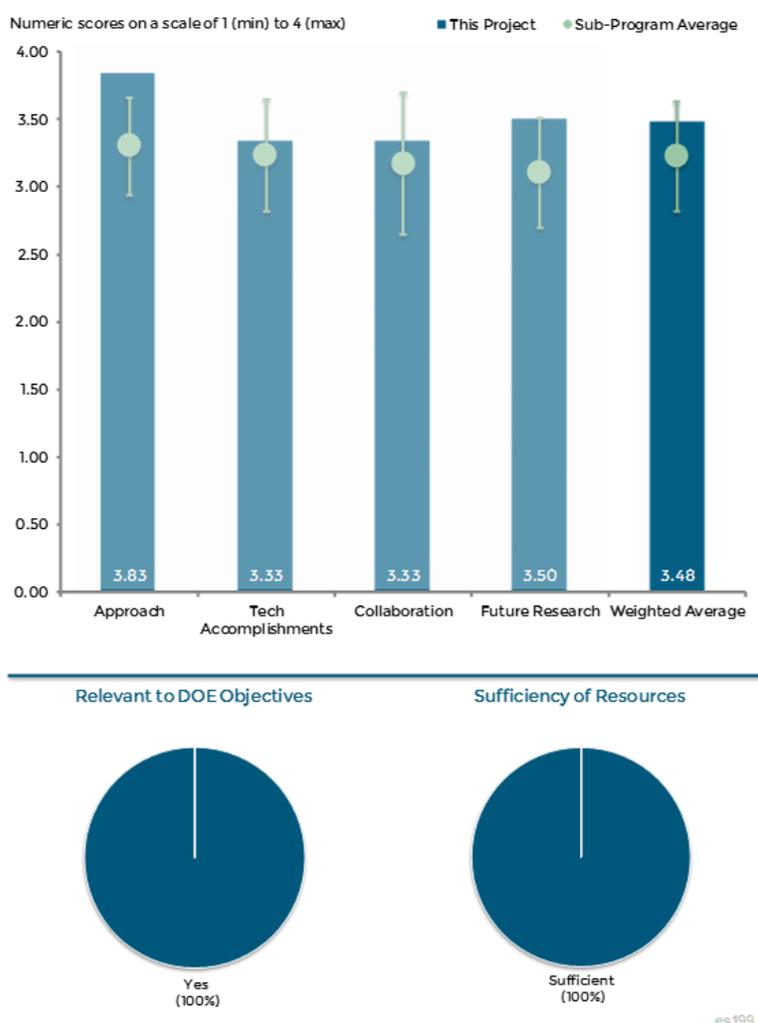


Figure 2-20 Coupling Mechanical with Electrochemical-Thermal Models Batteries under Abuse: Ahmad Pesaran (National Renewable Energy Laboratory) - Electrochemical Energy Storage

Reviewer 3:

The reviewer asked why the mechanical electrochemical-thermal (MECT) coupling relies on failure of the separator and subsequent contact of the anode and cathode as the failure mechanism. Noting that if the reviewer had interpreted the experimental data correctly, the mechanical tests indicated the separator is the most flexible material. In fact, the reviewer wondered, how did any of the mechanical measurements lead to input for the modeling studies, and vice versa. Are the groups working separately and then comparing results, the reviewer asked. The position of materials in the model was based on CT scans; the reviewer's question referred to the mechanical properties studies. A project goal includes improving the safety aspects of battery design. It was unclear to the reviewer how the results from this study would change the composition or design of a battery.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said the collaboration structure was very well defined and seemed to be working very well.

Reviewer 2:

The project is conducted by a very strong team consisting of industry and academic partners, the reviewer stated, with members working closely together.

Reviewer 3:

Noting that multiple institutions are involved, the reviewer found it hard to see if each group's studies relied on those of the others beyond the modeling partner relying on the CT images for structural input to the model.

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 goals of the project are well defined, the reviewer averred.

Reviewer 2:

The proposed future research is reasonable, the reviewer said, and agrees with the original plan, but alternatives to the solutions of the challenges and barriers seem not to have been addressed.

Reviewer 3:

The reviewer asked how MIT's models will be improved, noting that more specific details would have been helpful. The reviewer again raised the question of how, with respect to safer battery designs, the future work leads to improved cell designs.

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

Reviewer 1:

The understanding of multi-physics couplings on failure modes of electric vehicle battery components is critical to vehicle safety, the reviewer said, calling this a highly relevant project.

Reviewer 2:

The project will greatly aid future developmental efforts in new battery systems for advanced vehicle applications, the reviewer predicted.

Reviewer 3:

Safer battery designs will be helpful for the Li-ion battery market for plug-in electric vehicles (PEVs), 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:

It appears there are sufficient resources to achieve the proposed goals as planned, the reviewer felt.

Reviewer 2:

The reviewer recommended that, given the high financial cost of the project, the collaborators determine a way to pull up the schedule and complete the project within budget, suggesting that a no-cost extension of the schedule is appropriate if the allotted time is not sufficient.

Reviewer 3:

The only information suggesting excessive or insufficient funds was the delay in the disbursement of funds to one participant, the reviewer observed.

Efficient Safety and Degradation Modeling of Automotive Lithium-Ion Cells and Pack: Christian Shaffer (EC-Power) - es200

Presenter

Christian Shaffer, EC-Power.

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 technical barriers are well addressed in this project, said the reviewer.

Reviewer 2:

The prominent role of experimentation and use of hardware to inform software development is valuable, the reviewer stated. However, the materials, conditions and parameters incorporated thus far are somewhat limited, particularly in view of the planned project completion date in September 2015. Noting that a lot of time and effort have been devoted to the nickel cobalt aluminum oxide (NCA) database, the reviewer was surprised to see that only one cell nail penetration had been done to date.

Reviewer 3:

The approach is good for the portion of the project that was presented, in the reviewer’s opinion, although limited information was provided regarding the co-simulation with the structural mechanics module.

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 towards DOE goals.

Reviewer 1:

Much of the planned work has been accomplished except life testing, the reviewer observed.

Reviewer 2:

Limited validation was presented, the reviewer stated, and it was not clear whether the objectives could be adequately completed and meaningfully validated between the AMR and October. The incorporation of electrode swelling the reviewer regarded as a meaningful achievement. The model appeared to the reviewer to

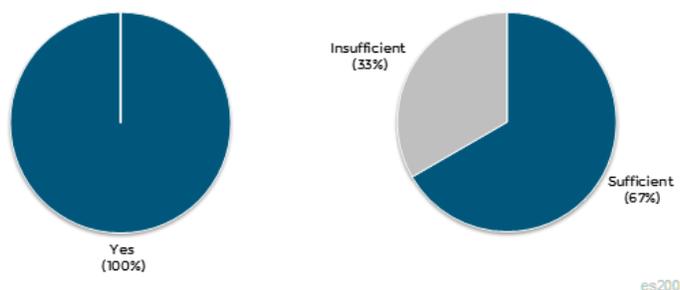
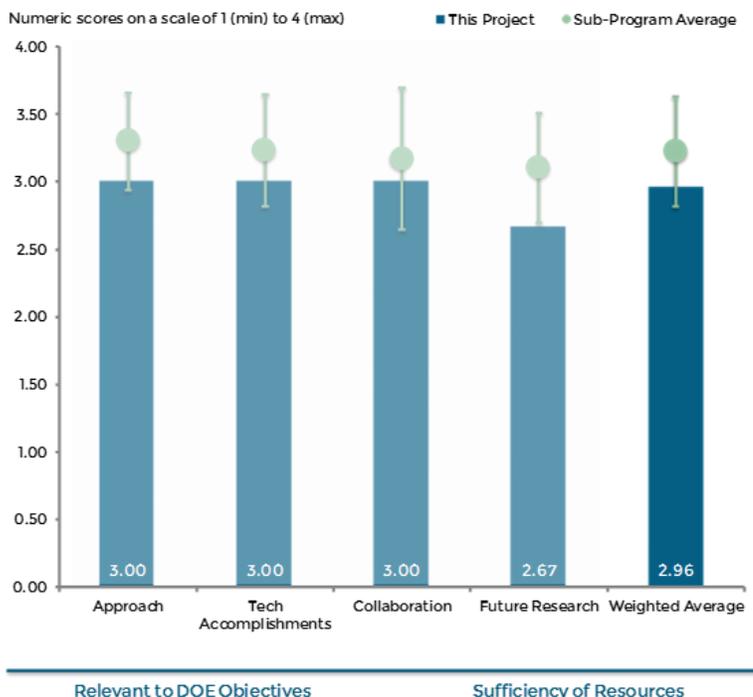


Figure 2-21 Efficient Safety and Degradation Modeling of Automotive Lithium-Ion Cells and Pack: Christian Shaffer (EC-Power) - Electrochemical Energy Storage

be less sophisticated than other works in this space, and the limited validation results shown did not, in the reviewer's opinion, show particularly good correlation between predicted and experimentally obtained values. Many of the significant milestones are scheduled for completion in October, which is when the project will be completed, and this seemed to the reviewer to be quite ambitious, allowing little time to accommodate contingencies.

Reviewer 3:

The results for the serial versus parallel connected cells provide good insight into physical mechanisms for failure and clarify the benefit of the development of such tools, in the reviewer's opinion

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The collaboration roles are clear, the reviewer said.

Reviewer 2:

The team members of the project have a good collaboration with each other, in this reviewer's view.

Reviewer 3:

The hurdles associated with fabricating large-format cells have negatively impacted the results, and will likely limit the amount of testing realistically achievable between May and program conclusion, the reviewer remarked, adding that this might have been more proactively addressed through identification of an alternate source for test fabrication and testing as soon as the problems were identified.

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 collaboration with a battery company to leverage their efforts in fabricating cells and/or batteries for model validation in order to save time.

Reviewer 2:

A significant amount of validation work remains that will be crucial for a meaningful project outcome, the reviewer noted, thus, prioritizing the amount of pack-level safety validation testing to validate the 3/8 cells in series and in parallel results would be useful.

Reviewer 3:

The reviewer asked that the co-simulation strategy with the structural mechanics module be clarified. Specifically, what is the technical plan (it was not fully described), and what example case studies will be explored to demonstrate the capability of the developed platform.

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

Reviewer 1:

This project supports the overall DOE objectives by developing battery safety and degradation models to aid battery design, the reviewer stated.

Reviewer 2:

EV battery safety is critical to promoting widespread adoption of highly efficient future vehicles, in the reviewer's opinion.

Reviewer 3:

While the goals are well-aligned with DOE goals, the reviewer said, output is inferior to that accomplished by other DOE-supported efforts in the same subject area domain.

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

Reviewer 1:

It seems, the reviewer said, there were insufficient primary or backup resources to execute the work plan. Noting that there are several months left, the reviewer conceded that observation might not be an accurate prediction, but believed that at present it was difficult to envision all milestones being achieved to the degree originally envisioned.

Electrochemical Performance Testing: Ira Bloom (Argonne National Laboratory) - es201

Presenter

Ira Bloom, Argonne National Laboratory.

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 PI has a long-standing reputation for highly focused, well-planned projects, the reviewer observed.

Reviewer 2:

The reviewer professed puzzlement as to why such extremes – 40% and 100%—were chosen for SOC, believing 90% would have been a reasonable target because this could be chosen to help prevent overcharge while using more of the battery capacity. Likewise, ending charging at 40% other than under exigency of time seemed unrealistic to the reviewer. The reviewer expressed interest in seeing the effect of testing to a set number of cycles at 40% SOC, then completing more at 100% SOC, rather than doing only 40% or 100%.

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 towards DOE goals.

Reviewer 1:

The reviewer praised the results achieved by this team as generally world-class, adding that the current data also reflect the meticulous nature of the test planning, execution and data analysis. However, the reviewer was puzzled by the disparity of test results from the Idaho National Laboratory (INL) and ANL who followed the same test protocols.

Reviewer 2:

The future work mentioned in the 2014 poster was addressed in 2015 and several factors were evaluated in fast charging experiments. The reviewer wondered if any publications resulted from this work.

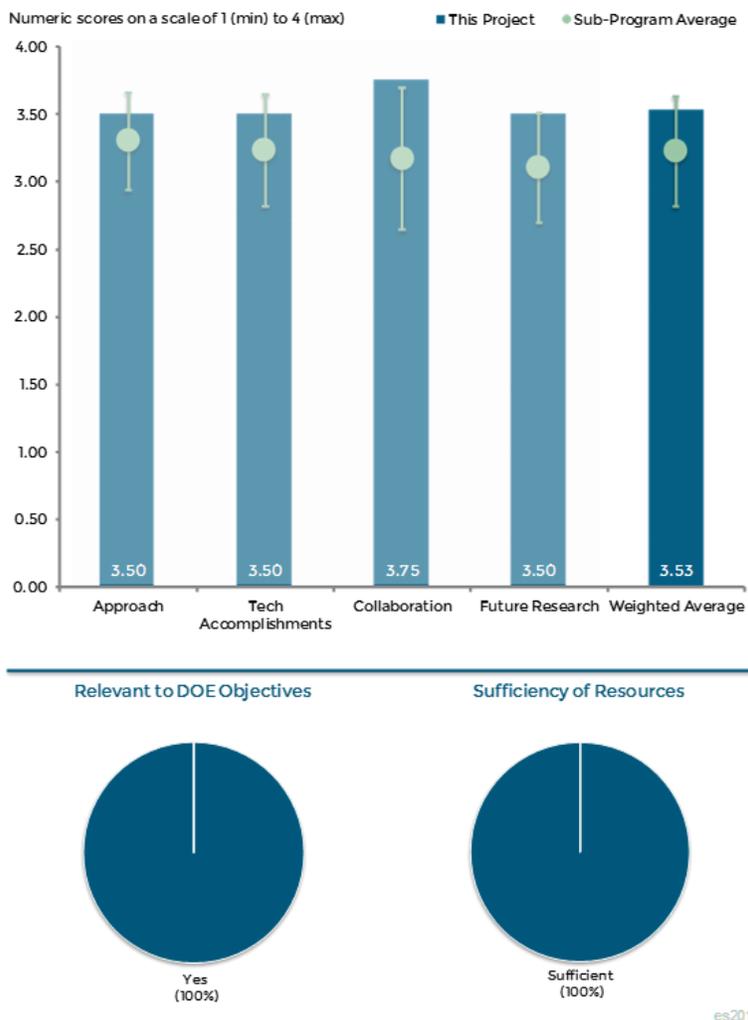


Figure 2-22 Electrochemical Performance Testing: Ira Bloom (Argonne National Laboratory) - Electrochemical Energy Storage

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

National laboratories are well known for collaborative work, the reviewer observed.

Reviewer 2:

The PIs are working with multiple companies and are comparing results with testing protocols used in China, was this reviewer's observation.

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 work plan is always well-thought out and thorough, said this reviewer.

Reviewer 2:

The project milestones provided were deemed inadequate by the reviewer. The reviewer considered that presenting test results at quarterly meeting does not include specific information on dissemination of results to the general public or scientific institutions. The Future Work slide in the presentation provides more useful information, but it is unclear when the work will be completed because the milestones only go through September 2015.

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

Reviewer 1:

Terming the project highly relevant, the reviewer praised the national laboratories as generally providing high-quality, unbiased evaluation of battery technologies.

Reviewer 2:

Improvement in battery performance would support their increased incorporation into EVs, decreasing the need, at least on a percent basis, for petroleum-fueled vehicles.

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

Reviewer 1:

The reviewer questioned the applicability of this question to national laboratories.

Reviewer 2:

It was unclear to the reviewer if any additional resources were needed to complete testing.

INL Electrochemical Performance Testing: Jon Christophersen (Idaho National Laboratory) - es202

Presenter

Jon Christophersen, Idaho National Laboratory.

Reviewer Sample Size

A total of two reviewers evaluated this project.

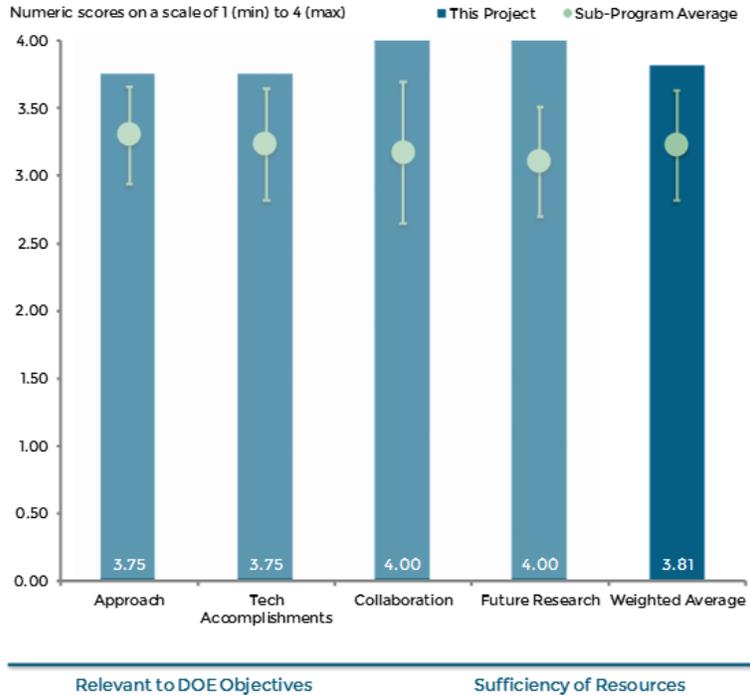
Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed, feasible, and integrated with other efforts.

Reviewer 1:

The approach is thorough, the reviewer said, the analysis of multiple performance factors allowing identification of the reasons for failure. Inclusion of vibrational monitoring adds a needed metric in evaluative tools, the reviewer added.

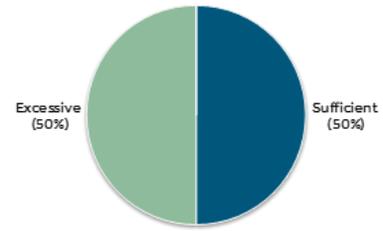
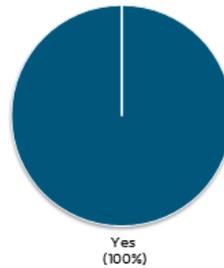
Reviewer 2:

INL has a long-standing reputation for highly focused, well-planned projects, the reviewer stated.



Relevant to DOE Objectives

Sufficiency of Resources



es202

Figure 2-23 INL Electrochemical Performance Testing: Jon Christophersen (Idaho National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

Praising the project team for its routine execution of high-quality testing studies, the reviewer added that their contribution to the generation of world-class testing protocols/manuals can hardly be overstated. The results of life modeling using real-life data over a long period of time are very valuable, the reviewer concluded.

Reviewer 2:

The reviewer called the publication of manuals and patents impressive, but would have liked to have seen contributions to the peer-reviewed literature and considered that this seemed like a great opportunity to reach the broader public as well, perhaps through collaborative publications with science writers. The reviewer was unsure, however, if that is something DOE requires through this funding mechanism.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Collaboration with many other institutions, in the form of testing the performance of other institutions' batteries, the reviewer said, is clearly evident and abundant.

Reviewer 2:

The reviewer noted extensive collaboration with various laboratories and organizations.

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:

Testing of articles that were used to predict life, the reviewer urged, should be continued as long as possible to generate a robust baseline data set.

Reviewer 2:

The reviewer asked why the Tech-to-Market workshop is limited to industry. The reviewer expressed the belief that researchers from national laboratories and academia, too, could benefit from learning about testing protocols. The reviewer speculated that perhaps there is another outlet through which this information could be disseminated.

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

Reviewer 1:

Absolutely, the reviewer said; INL is an integral part of battery development process/testing.

Reviewer 2:

By providing analysis to national laboratories and companies on performance metrics, the projects' PIs are enabling more reliable data for performance that may lead to better integration of lithium-ion batteries in the battery market, the reviewer stated.

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

Reviewer 1:

While noting that many channels are available, the reviewer wondered if even more progress could be made by further equipping the facilities with more channels and temperature-controlled chamber(s).

Reviewer 2:

Unless the funds are used to procure/upgrade equipment, the reviewer said, they seem to be a bit on the high side.

**Battery Safety Testing:
Christopher Orendorff (Sandia
National Laboratories) - es203**

Presenter

Christopher Orendorff, Sandia National Laboratories.

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 commented on the project’s very well-organized, focused work plans and noted that SNL meticulously carried out planning for testing of DOE-sponsored research articles.

Reviewer 2:

The work is thorough and diverse, the reviewer said, noting the failure propagation test and car crash-worthiness studies with particular approval. The reviewer further noted the PI’s response to reviewer comments about the difficulty in predicting failure response, saying it was reasonable and pointing out that the project team had to start somewhere.

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 towards DOE goals.

Reviewer 1:

The reviewer deemed the results to be benchmarks in the industry. Tests such as failure propagation, for example, still engender considerable controversy surrounding methods, the reviewer observed, suggesting it might be worth pursuing multiple options to evaluate the pros and cons of the various methods.

Reviewer 2:

Many setups deliver a variety of performance testing abilities, the reviewer said, adding that the combination of modeling with experiment is appropriate and should be continued. The reviewer expressed support for the evaluation of cells from multiple manufacturers.

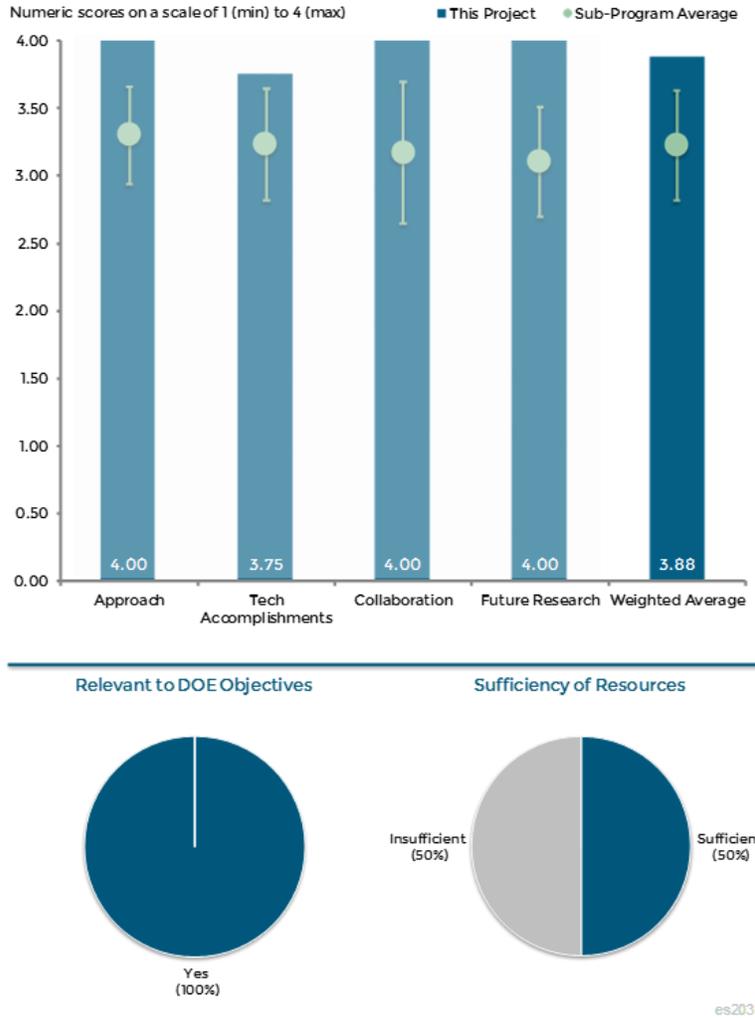


Figure 2-24 Battery Safety Testing: Christopher Orendorff (Sandia National Laboratories) - Electrochemical Energy Storage

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Testing includes multiple institutions and companies in all project areas, the reviewer observed, and the collaborative efforts are reflected in the authorship of resulting publications.

Reviewer 2:

Noting extensive collaboration with various organizations and labs, the reviewer suggested that an important partner could be Chinese national laboratories in order to exchange, develop and harmonize test protocols.

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:

Given the current emphasis on development of Li metal-based systems, the reviewer said, it will be instructive to include and benchmark the abuse tolerance of Li metal battery systems such as those commercially available from Sion or Bolloré. The reviewer suggested collaboration with Chinese national laboratories.

Reviewer 2:

The proposed future research seemed reasonable to the reviewer based on results obtained to date. However, the reviewer found the specifics of the proposed research difficult to critique due to the amount of detail provided.

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

Reviewer 1:

SNL's role in DOE's efforts to develop better batteries to displace petroleum cannot be overstated, the reviewer emphasized.

Reviewer 2:

Improving performance and understanding of performance and failure in Li-ion batteries may allow for improved battery design and/or management systems to create more reliable systems, the reviewer suggested. The reviewer concluded that preventing failure may lead to increased incorporation of Li-ion batteries into EVs, a factor critical to the displacement of petroleum.

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

Reviewer 1:

Considering how costly abuse-testing studies are, the reviewer was unsure the current level of funding is sufficient.

Reviewer 2:

The laboratories have set up systems to test multiple aspects of performance and failure and seem to have made good use of the resources allocated for them, the reviewer said.

Battery Thermal Characterization: Matthew Keyser (National Renewable Energy Laboratory) - es204

Presenter

Matthew Keyser, National Renewable Energy Laboratory.

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 complimented the project work plan as well-planned and well-focused.

Reviewer 2:

Noting that the PIs had measured thermal and electrochemical performance of Li-ion batteries, the reviewer found it difficult to see how the individual experiments are related, acknowledging that this difficulty might result from a lack of familiarity with the project team’s specific research. All experiments seem to involve temperature and cycling, the reviewer observed, but questioned whether one experiment leads to another, for example, or multiple experiments are combined for a more thorough understanding. The reviewer also believed it would have been expected before any of these tests were done that improperly designed thermal management systems can lead to a cell-to-cell temperature spread. The reviewer also expressed an interest in knowing what cell chemistries were tested as far as typical and new chemistries have been noted.

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 towards DOE goals.

Reviewer 1:

The high-quality thermal studies data NREL presented are extremely useful to the developers, the reviewer stated. The reviewer also noted the unique calorimeter the project team have developed, its size in particular, calling it a valuable tool for characterizing cells of varying sizes and shapes. Thermal imaging, efficiency and entropic data are valuable parameters for the researchers, the reviewer concluded, calling NREL the go-to lab for procuring reliable thermal data.

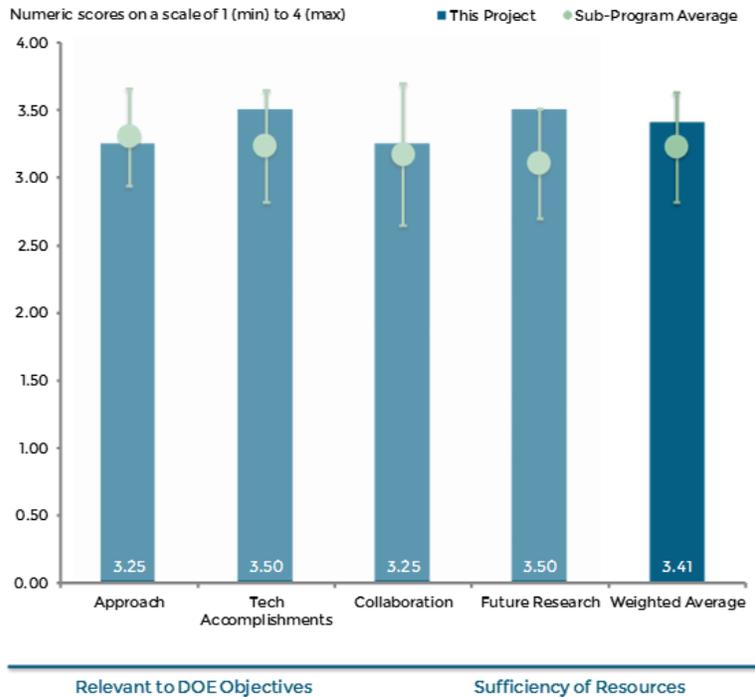


Figure 2-25 Battery Thermal Characterization: Matthew Keyser (National Renewable Energy Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer found the entropic studies quite interesting to learn about, but was unsure how that will lead to improvements in design. The reviewer also noted that publications in peer-reviewed literature were not included in the list of accomplishments, asking if this was not important for the project.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer discerned excellent collaboration with various laboratories and organizations.

Reviewer 2:

While several partners were listed, the reviewer noted, it was not clear how the PIs are working with those partners. For example, the reviewer said, it was unclear if the PIs are testing batteries from all or some of the 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:

Pack-level studies using the OEM drive-profiles will be very interesting, the reviewer predicted, suggesting the possibility of characterizing cells/packs at end of life.

Reviewer 2:

The reviewer wondered how the PIs propose to reduce cell-to-cell temperature variations. Learning there are thermal variations does not necessarily lead to the conclusion that a solution to temperature variation is the next step. The reviewer asked whether work with room-temperature refrigerants means that the next year will involve thermal analysis when liquids are surrounding battery exteriors. If so, the reviewer questioned how the temperature of the battery itself will be measured, rather than that of the liquid.

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

Reviewer 1:

Affirming that the project is supportive of DOE's petroleum replacement goal, the reviewer called thermal characterization and modeling important for the development of efficient cells/batteries.

Reviewer 2:

The information developed in the project may lead to better batteries for PEVs, 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 funding level seemed appropriate to the reviewer.

Reviewer 2:

No deficiency in results is apparent, the reviewer said.

New High-Energy Electrochemical Couple for Automotive Applications: Khalil Amine (Argonne National Laboratory) - es208

Presenter

Khalil Amine, Argonne National Laboratory.

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 approach seemed very comprehensive to the reviewer, who noted the anode, electrolyte and cathode were all combined to achieve a high-energy battery, with long calendar and cycle life. The project team are strongly focused on the critical barriers, the reviewer concluded.

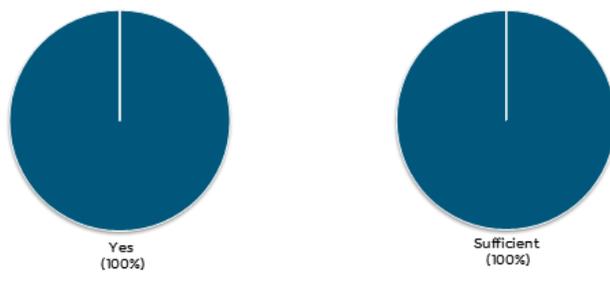
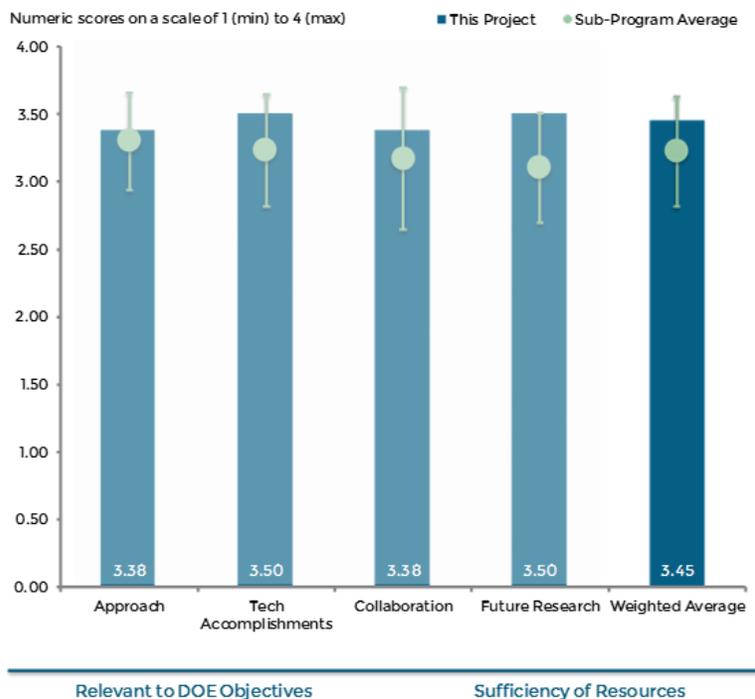
Reviewer 2:

The FCG materials seem to be a viable approach to increase the lifetime and capacity of NMC-based materials. The reviewer termed the cathode part of the project impressive and said the combination of high-resolution analytical techniques and electrochemical investigations proves the concept very well. The reviewer welcomed the use of SiO-SnCoO as anode material as opening an alternative to the commonly used Si/Si-C material.

The anode material target of 900 mAh/g, the reviewer said, can be sufficient for the DOE PHEV-40 target. It would be of additional benefit, the reviewer concluded, to investigate the potential of the material to exceed 1,000 mAh/g and thus also to address EV application.

Reviewer 3:

The full concentration gradient (FCG) cathode material appears to be far ahead of the Si-based material development, the reviewer noted, which appeared to be reflected in the basic understanding of the system. The reviewer continues to be concerned that with all the work on multiple Si-based systems – not just that presented here – there appeared to be a fairly significant lack of fundamental understanding around the material sets. This, the reviewer went on, is not a concern regarding the present work in this data, but all work associated with these materials.



es208

Figure 2-26 New High-Energy Electrochemical Couple for Automotive Applications: Khalil Amine (Argonne National Laboratory) - Electrochemical Energy Storage

Reviewer 4:

The key barriers that must be addressed, the reviewer stated, is long calendar and cycle life, but it is not clear how to address this challenge. In particular, the reviewer said, a solution for the instability of the SEI layer and attack by dissolved Mn from the surface of the FCG cathode to the anode side were not clearly discussed or planned. Also, the current anode system shows poor capacity and cycle life, problems the reviewer said could not be solved by addressing only the binder.

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 towards DOE goals.

Reviewer 1:

The reviewer called the progress of the work within the past year quite impressive, showing the project team's effective and target-oriented way of working. The scientific approach and experimental methods, the reviewer said, are well chosen and the evaluation of the best binder option was very interesting. The capacity and cycling stability of the cathode material could be well improved, in the reviewer's view, but a capacity above 200 mAh/g could only be reached at 4.5 V with negative impact on cycle life. The capacity advantage disappeared after 50 cycles and might be even worse at higher cycle numbers, the reviewer said. At present, the reviewer observed, FCG has a mean composition of 622 to adjust to the 622 baseline, but recommended that Ni content be increased in the next step to meet the target. For the anode alloy with optimized binder LiPAA, good cycle life was shown for alloy contents of 33%, the reviewer noted, which does not lead to the targeted capacity. The reviewer recommended adding an investigation of cycle performance as a function of alloy content. The reviewer concluded by calling attention to a table in the presentation showing the BatPaC cell design results and recommended adding a line with the DOE cell targets and an additional baseline 622 versus graphite to show the different effects of new anode and cathode materials.

Reviewer 2:

The reviewer found the thermal stability data on the NMC 622 FCG very compelling, adding that it is easy to understand that as the Mn content increases toward the surface of the particles, the powder will be more stable. However, the reviewer continued, higher-than-baseline capacity of the gradient powder reported by the authors appears more difficult to understand. The reviewer speculated that there could be small fluctuations in the overall Ni content of the two cathode powders, with the gradient material having a little more Ni. Poor distribution of the negative active material associated with the electrode processing of the anode (SiO-SnCoC-MAG) seems a reasonable explanation for the poor performance in a full cell, the reviewer concluded.

Reviewer 3:

As the reviewer noted earlier, there appeared to have been solid progress made on the FCG material, but less on the Si material.

Reviewer 4:

The reviewer noted good progress, although the cycle life of the anode side still needs significant improvement. For the cathode, the reviewer said, optimization may be achieved further by considering particle size and grain structure. The reviewer observed that no detailed study on rate capability was done and that there was discussion of abuse tolerance even though that is one of barriers it was desired to address.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

Collaboration with other institutions seemed very good to the reviewer, who noted that they complemented each other.

Reviewer 2:

The collaboration is well balanced and seemed to work effectively, in the reviewer's opinion. The reviewer voiced the expectation that the focus of the different partners will be continuously adjusted to the findings, for example to results on binder or anode electrode processing.

Reviewer 3:

Noting the presence of several partners in the overview slides, the reviewer said the outcome of the SEI and facility scale-up were not shown.

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 termed the project team a solid group of high-quality contributors.

Reviewer 2:

After an independent confirmation of a better electrochemical performance, including capacity, for the gradient powders is achieved, the reviewer said, strong efforts should be directed toward a scale-up of the production process. The authors mentioned the production of one kilogram of cathode powder per batch, leading the reviewer to wonder if the process is scalable to 500 to 1,000 kg.

Reviewer 3:

The proposed next steps, the reviewer said, address the present challenges or missing results. The reviewer also directed attention to earlier comments on future work included in the Comments on Technical Accomplishments and Progress section.

Reviewer 4:

Abuse tolerance must be added in the future plan, the reviewer urged, as it was not discussed or addressed in spite of being one of the key target elements.

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

Reviewer 1:

The project is strongly related to the objective of petroleum displacement, the reviewer stated, because stable, high-energy cathode powders are very important in this area.

Reviewer 2:

The reviewer called higher-energy-density cells obvious targets for DOE objectives.

Reviewer 3:

The work is aimed at achieving a higher battery energy density necessary to increase the range and market chances for future PHEVs and EVs, the reviewer observed.

Reviewer 4:

Development of high cathode and anode is essential for enabling PHEVs and EVs, according to this reviewer.

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

Reviewer 1:

If the authors plan to scale up the processes, the reviewer qualified, the resources are not sufficient.

Reviewer 2:

The reviewer observed that budgets were not broken down by individual investigator efforts.

High-Energy High-Power Battery Exceeding PHEV-40 Requirements: Jane Rempel (TIAX) - es209

Presenter

Jane Rempel, TIAX.

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 project team is well focused on the critical areas and should overcome most barriers. It was apparent to the reviewer that that the authors have managed to overcome potential difficulties associated by working with critical suppliers.

Reviewer 2:

The reviewer commented that the approach appears to be to use a fairly well characterized and well performing cathode material (CAM-7 in this case) and matched it with Si-based anode

structures that have been provided as potential counterpart anode electrode structures. The reviewer noted that with every reviewed cathode/Si anode proposal, there appears to be a lack of fundamental understanding and development around the Si anode limitation, which is concerning. The reviewer opined that there is certainly a place for this work being performed, and there is nothing wrong with it, but also noted that the key to making any of these designs work appears to be in the Si side of the equation.

Reviewer 3:

The reviewer noted that the principal approach in terms of set of material is reasonable and similar to the comparable projects, but there are no details disclosed on how to further develop the material properties in order to meet the targets.

Reviewer 4:

The reviewer expressed that the uniqueness of the project was not very clear because it seems the team relies significantly on the vendors and that the presentation slides do not represent the actual research activity. For example, hard C, which was not actually used. The reviewer also noted that the slide and presentation information do not convey detailed technical discussions.

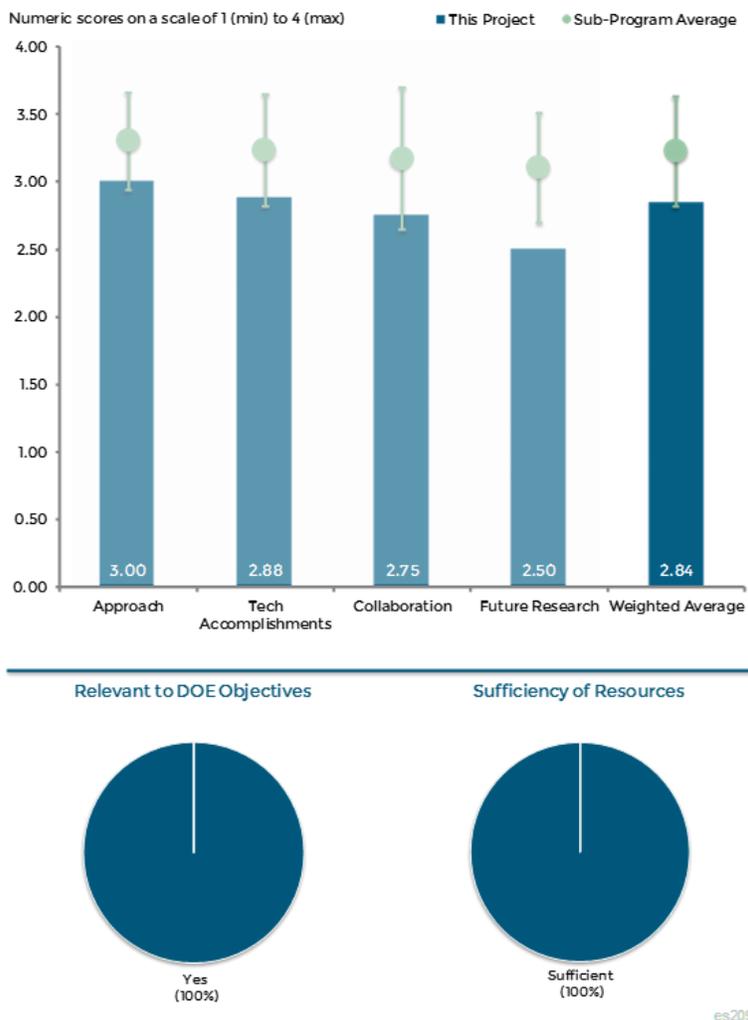


Figure 2-27 High-Energy High-Power Battery Exceeding PHEV-40 Requirements: Jane Rempel (TIAX) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer said that it will be interesting to see the specially designed set-up used to monitor the rise in internal cell pressure due to the silicon anode. Slide 6 shows the specific capacity obtained using a low-loading electrode. The reviewer suggested that at some point, the authors should mention the electrode loading to better judge its performance for it could be of interest to know how reproducible is the data obtained from different batches of cathode powder.

Reviewer 2:

The reviewer observed that the graphite/CAM-7 work appears to be performing as it should which is fine, but is a somewhat mature data set which is not necessarily in need of development funding. The reviewer also noted that the Si-based cell has baseline promise, but the key to further progress really lies on the Si materials developers.

Reviewer 3:

The reviewer commented that for the graphite material, the capacity retention looks good, but, 1 Ah at C/20 discharge rate is low compared to the commercial products. However, the reviewer pointed out that the Si cell shows poor cycling performance.

Reviewer 4:

The reviewer noted that the milestone overview between 2014 and 2015 is unchanged where it just states scheduled and it is unclear which milestones are completed. The baseline cell (CAM-7/Graphite) with a cathode loading of 2 mAh/cm² and 1.8 ampere-hour (Ah) for an 18650 cell is quite low compared to the state of the art. The reviewer also stated that the cycling data of the baseline cell seems to be the continuation of the cycling test shown in 2014, but the capacity retention of the 2014 and 2015 curves, in regards to DOE, does not fit. There is no information given regarding a further improvement of the baseline cell. The reviewer observed that most of the presentation shows results of the baseline cell. No information is given regarding material and/or electrode development.

The reviewer added that the achieved capacity of 2.85 Ah with a cathode loading of 4 mAh/cm² can be achieved with graphite where to compare baseline cell with 1.8 Ah and cathode loading 2 mAh/cm², and that an improvement by the Si based anode is not obvious. The reviewer expressed that the pressure variation during cycling is a good experiment, but it is difficult to interpret as the amount of Si in the anode and the packing density of the jelly roll within the 18650 cell is not given. As the capacity is not too high, it is assumed that the pressure build up could be substantially higher when the cell volume is better utilized.

The reviewer also noted that the capacity fade within 30 cycles is by far too high. No explanations regarding root cause or measures to improve are given. Additionally, the reviewer remarked that the details in presentation es260 are quite general and cannot be linked to the open issues mentioned above.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

It was apparent to the reviewer that the project team has a good collaboration with the suppliers. As explained on Slide 20, in future projects, the team is planning on having a stronger collaboration with DOE laboratories.

Reviewer 2:

The reviewer stated that the project work is done without collaborative partners. The level of material supplier input regarding knowhow and analysis cannot be judged and is also not obvious in the results.

Reviewer 3:

The reviewer said that there is no collaboration except for material suppliers. Also, no details are provided for the interaction with collaborators.

Question 4: Has the project 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 was apparent to the reviewer that the authors are overcoming most barriers. Gen 1 CAM-7/Si cells are providing power and higher energy density on 18650 cells. The reviewer pointed out that the limiting factor is the capacity retention of the Si-containing anodes. Blended anodes or pre-lithiation are mitigating strategies. The reviewer suggested the team to scale up initiatives of the CAM-7 high-energy and that high power cathode should be addressed in the future.

Reviewer 2:

The reviewer commented that the project team should continue to optimize the design of Si anodes and opined that this project has been going on for a long time.

Reviewer 3:

The reviewer said that the next steps do not disclose the technical actions to be taken. Taking into account the present low cycle life of the target cell, the achievement of the final project goals is questionable.

Reviewer 4:

The reviewer stated that there are no specific plans for improving cycle life, calendar life, and temperature range, which are all described in the overview slides.

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

Reviewer 1:

The reviewer confirmed that the project team is very focused on the development of high-capacity Li batteries, which is very much aligned with petroleum displacement.

Reviewer 2:

The reviewer expressed that high-energy density cells clearly relate to the U.S. Department of Energy (DOE) objectives.

Reviewer 3:

The reviewer remarked that the development lithium-ion battery systems that meet and exceed the PHEV-40 performance and life goal is necessary for achievement of DOE objectives.

Reviewer 4:

The reviewer stated that the work is aimed towards achieving a higher battery energy density necessary to increase the range and market chances for future PHEVs and EVs.

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 not much is said about the working relationships with the material suppliers and maybe the resources are not sufficient.

Reviewer 2:

The reviewer stated that detailed budget information is not available.

Advanced High-Energy Lithium-Ion Cell for PHEV and EV Applications: Jagat Singh (3M) - es210

Presenter

Jagat Singh, 3M.

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 concluded that the approach is good leaning to excellent. As will be seen in collaborator section, at least this work has subject specific experts contributing in all major fields of concern.

Reviewer 2:

The reviewer said that it is encouraging that nanostructure-based Si alloy anode and advanced cathode both demonstrate improvement in capacity as cycling number increases. However, the demonstrated cycle number is not sufficient for commercialization. The reviewer pointed out that another concern is the structural instability due to mismatch for the core shell cathode material.

Reviewer 3:

The reviewer expressed that the approach is reasonable and comparable to similar projects.

Reviewer 4:

The reviewer noted that the advanced cathode development seems very interesting, in particular, the NMC 622. However, even though the presentation showed improvements, it is not very clear about the deliverables.

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 towards DOE goals.

Reviewer 1:

The reviewer noticed that, as with other programs of this type, and there are several, the cathode technology is far ahead of the anode technology. The reviewer is in favor of all advanced design data sets as compared to a cathode/graphite control cell. 3M Company is a long time developer of Si anode material and has a strong

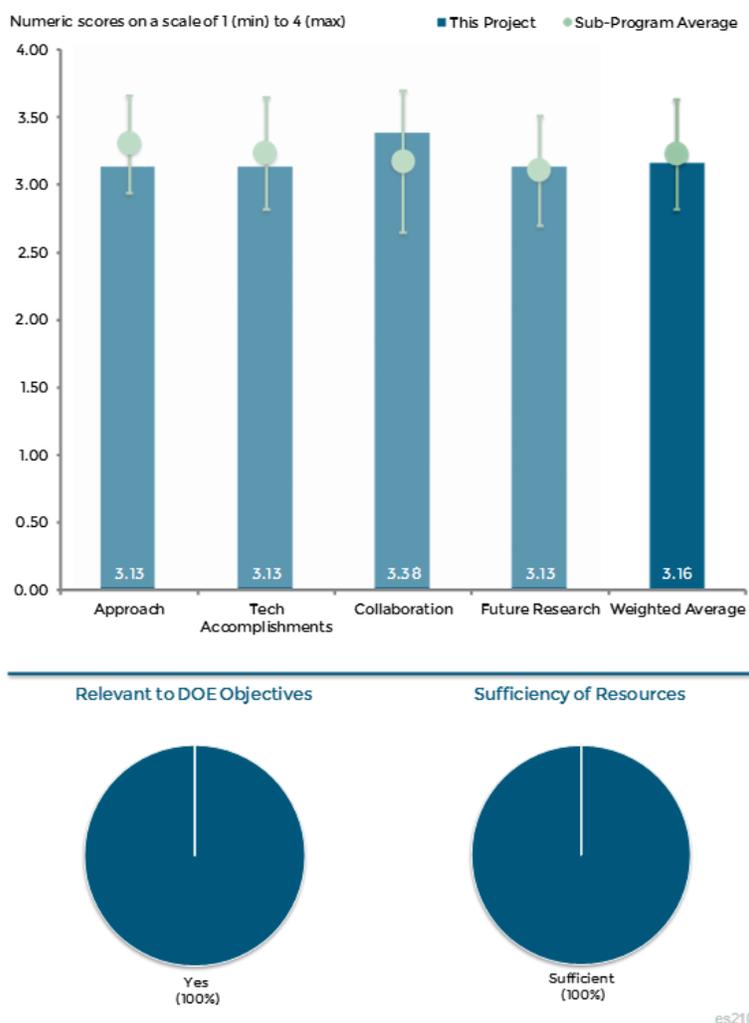


Figure 2-28 Advanced High-Energy Lithium-Ion Cell for PHEV and EV Applications: Jagat Singh (3M) - Electrochemical Energy Storage

commercial focus. Understanding where the technology compares to state of the art baseline, for example graphite, seems reasonable to the reviewer as a comparison to make.

Reviewer 2:

The reviewer stated that the authors managed to produce advanced anode and cathode materials of higher capacity. Cycle life improvement with additives one and two seems impressive; however not much information is provided. Similarly, the reviewer noted that with the high-voltage NMC cathode in Slide 8, the new NMC cathode powder seems to double the cycle life.

Reviewer 3:

The reviewer expressed that the demonstrated rate capability is still not sufficient in terms of cycle life and C-rate. The improvement must be demonstrated over 1,000 cycles to be competitive commercial product, and the technical issue and surface stability must be addressed to achieve the target.

Reviewer 4:

The reviewer noted that the improvements in the Si-alloy anode shown are minimal and far from target, from 66% to 70% capacity retention after 500 cycles. Moreover, testing conditions like voltage and C-rate are not given. For the cathode material capacities above 200 mAh/g are only reached at high-voltage of 4 and/or 6 V. Accordingly it shows high-capacity fade of 20% after 100 cycles. The reviewer pointed out that the slide regarding the core shell material from partner, Umicore, is misleading as it is not the material used in the previous chart and in the subsequent full cell tests, for the composition, in regards to DOE, does not match. Test of electrolytes and additives are done with different test conditions such as room temperature (RT), C/5 discharge rate versus 30° Celsius (C), C/3 discharge rate.

The reviewer recommended harmonizing the test conditions, and the cycling test for the additives stops at 75 cycles. It can be expected that even the best option (i.e., additive 1 + additive 2), will fall off with increasing cycle number. The reviewer's recommendation is to extend the cycling tests. Results in 18560 cells are referred to advanced chemistry but no explanation is given of the material optimizations. Moreover, just the rate capability is shown, where the most important would be the cycling performance.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team has a very good collaboration set and the reviewer expressed an appreciation of the data provided.

Reviewer 2:

The reviewer stated that the project team's collaboration seems to be very good which includes universities, companies, and national laboratories.

Reviewer 3:

The reviewer remarked that project partners are well recognized companies or laboratories with high competence in the field and are able to address all relevant challenges. However, the progress shown, in regards to DOE, does not fully reflect this strong partnership where a close interaction between the partners was not obvious from the available material. The reviewer concluded that it is recommended to strengthen the interaction.

Reviewer 4:

The reviewer observed that there is a good project team collaboration with strong multidisciplinary teams. However, the challenges for multiple organizations, such as lack of effective communications and feedback updates, must be resolved. The reviewer states, for instance, sample preparation, electrolyte, binder, optimization, evaluation/analysis are all conducted in different research groups, and how effectively the teams communicate and exchange the data will be an issue.

Question 4: Has the project 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 efforts to scale-up cathode and anode materials is going to be important at the cell level. However, in future presentations, the reviewer expressed that the authors should give some idea on how scalable the production processes are for a more massive production of those powders.

Reviewer 2:

The reviewer mentioned that principal direction of future research is reasonable, but taking the remaining time into account seems to be critical to reach the targets, and expressed that it would be desirable if a more detailed action plan were established for the last few months.

Reviewer 3:

The reviewer commented that a plan for cycle life improvement is not included in detail, and especially concluded that the mechanical failure and SEI layer instability must be addressed.

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

Reviewer 1:

The reviewer pointed out that yes, the project is focusing on the delivery of high-capacity batteries that, at some point, could be used for electric propulsion, and this is much related to petroleum displacement.

Reviewer 2:

The reviewer observed that high-energy density cells are obviously in the interest of the DOE objectives.

Reviewer 3:

The reviewer expressed that advanced a high-energy Li-ion cell for PHEV and EV applications is urgently needed for achieving the DOE objectives.

Reviewer 4:

The reviewer stated that the work is aimed towards achieving a higher battery energy density necessary to increase the range and market chances for future PHEVs and EVs.

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

Reviewer 1:

The reviewer observed that the project is almost complete at his time, and the team made substantial progress, but cycle life could be a challenge.

Reviewer 2:

The reviewer noted that the costs were not broken down by individual efforts.

High-Energy Lithium Batteries for PHEV Applications: Subramanian Venkatachala (Envia Systems) - es211

Presenter

Subramanian Venkatachala, Envia Systems.

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 praised that the approach has some fundamental analysis of the direct current (DC) resistance rise of the cathode material, as for in most of these presentations, the Si anode portion of the approach is more of an afterthought and really needs to occur within a dedicated program.

Reviewer 2:

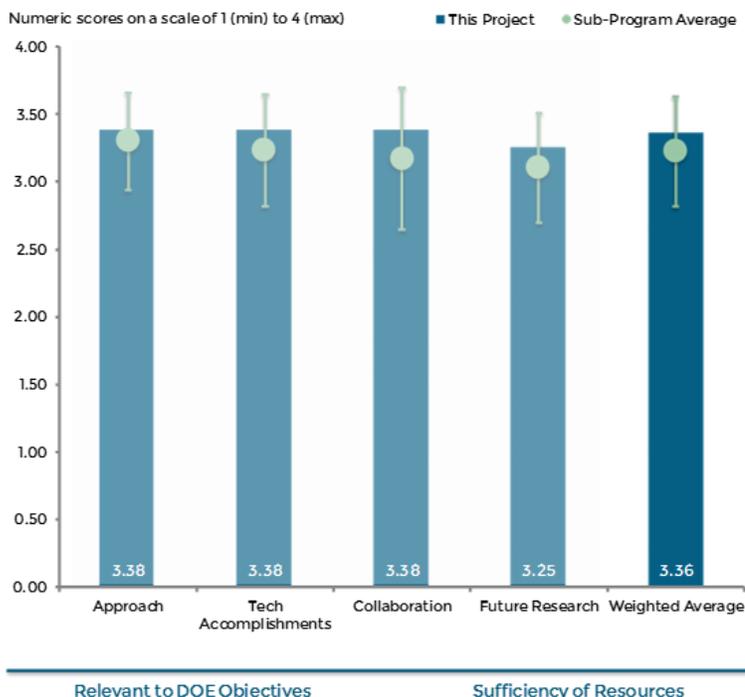
The reviewer pointed out that the approach is sharply focused in the critical areas, where the transition from HCMR-XLE towards HCMP-XE seems appropriate based on the experimental evidence.

Reviewer 3:

The reviewer pointed out that the strategy based on root cause is well organized. However, the focus should be made based on analysis, and not trial and error. The reviewer expressed that the atomic layer deposition (ALD) coating, competition between mechanical stability, and species transportation that may be hindered by thick layer, must all be considered and optimized.

Reviewer 4:

The reviewer noted that the technical approach in the particular coating of the Mn-rich material is reasonable. The necessary high capacities above 200 mAh/g are only achieved within the large voltage window between 4.6 and 2.0 V, where the high upper cutoff voltage and the quite low mean voltage might be disadvantageous, and thus, the cycle life for the first and energy density for the latter.



es211

Figure 2-29 High-Energy Lithium Batteries for PHEV Applications: Subramanian Venkatachala (Envia Systems) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer opined that the cathode progress was quite interesting.

Reviewer 2:

The reviewer noticed that due to the well-structured and scientifically sound way of working, the project team has made substantial progress in the past year, and expressed appreciation that the results were shown in reasonable detail, even when the approach was not successful. When looking at the cathode material results, it is questionable whether the open challenges including structural phase changes can be solved. Moreover, the large voltage span is an additional challenge. The reviewer added that regarding the anode material, it is not obvious that there is a substantial in-situ graphene production, and moreover, in the case that graphene is produced, it improves the performance, but only 40 cycles were shown. It is recommended to show the presence of graphene experimentally and analytically and present a model of how this increases the performance and/or the lifetime. The reviewer said that the results on the binder investigations were interesting and give good hints for the direction of future work. The full cell testing of high capacity manganese rich (HCMR) graphite shows quite good cycling but at substantial lower voltage than 4.4 V as compared to the results shown for the material development. The reviewer concluded that only capacities below 200 mAh/g are achieved and are also possible with Ni-rich NMC for example, and that it is recommended that the project team make a critical evaluation of the particular HCMR approach at the end of the project.

Reviewer 3:

The reviewer acknowledged that the authors have done an appreciable amount of work with different types of coatings on the cathode powders, and it seems that the formation of the spinel like structure will always develop as the material is cycled. The reviewer mentioned that project team should probably do some temperature stability studies on their cathode powders in the future.

Reviewer 4:

The reviewer noted that even though using XE versus graphite shows good results, it should be extended to high-energy anode material, and the explanation for observed phenomena must be made to utilize the observed results.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that the project team has very good collaboration with other institutions, such as Lawrence Berkeley National Laboratory (LBNL) and General Motors.

Reviewer 2:

The reviewer remarked that the project team collaboration is small but with competent partners, and thus, allows effective cooperation with the partners who seem to well coordinate their efforts, which is leading to good results.

Reviewer 3:

The reviewer commented that the work appeared to be very seamless, but could not tell from the presentation who did what, so unfortunately could not comment on the collaboration execution.

Reviewer 4:

The reviewer mentioned that the project team collaboration involves many organizations and researchers, but an effective communication approach must be established.

Question 4: Has the project 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 project team's proposed future work, the design of large format cells of high-energy with the incorporation of Si-anodes, is the right approach now that the project is reaching completion.

Reviewer 2:

The reviewer observed that the proposed future work on selecting final coating, as well as further detailed analytical work to disclose fundamental mechanisms, is well structured. From the previewed results, it is questionable whether further coating attempts, as described in the Future Work, will be successful, in particular as there is only little time left. The reviewer added that due to the remaining open questions, it seems critical to reach the project targets on cell level. It would be desirable to have more detailed action items on target cell level and a forecast of expected final performance.

Reviewer 3:

The reviewer commented that the project team's proposed future work needs to have some cost guidance put into the future research direction.

Reviewer 4:

The reviewer pointed out that the most significant challenge is to use Si material in this project, but most of the current work is focused to the cathode materials. The project teams need to set up a clear and specific plan for addressing anode materials.

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

Reviewer 1:

The reviewer said that the work is very relevant to the overall DOE objectives. The development of high-energy batteries is at the core of the petroleum displacement objective.

Reviewer 2:

The reviewer stated that the high-capacity cell designs are an important piece of vehicle electrification.

Reviewer 3:

The reviewer observed that the work is aimed towards achieving a higher battery energy density necessary to increase the range and market chances for future PHEVs and EVs.

Reviewer 4:

The reviewer noted that enabling the use of the high-energy offered by Li-rich cathode material is essential for achievement of 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 acknowledged that the project team is almost at the end of the program, and based on the data and the amount of work performed, the resources were well utilized.

Reviewer 2:

The reviewer noted that the budget is not broken down for individual effort.

High-Energy, Long Cycle Life Lithium-Ion Batteries for PHEV Applications: Donghai Wang (Pennsylvania State University) - es212

Presenter

Donghai Wang, Pennsylvania State University.

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 explained that the technical approach shows a very good understanding to improve properties step-by-step towards the target. The path to the project cell is systematically planned.

Reviewer 2:

The reviewer stated that the author tried to focus in many different areas to produce a higher energy battery. The problem was attacked from multiple fronts, such as new energy cathodes, electrolytes, electrolyte additives, coatings, and Si/Si alloy-C electrodes.

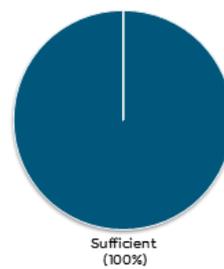
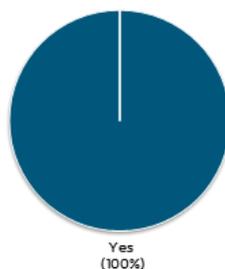
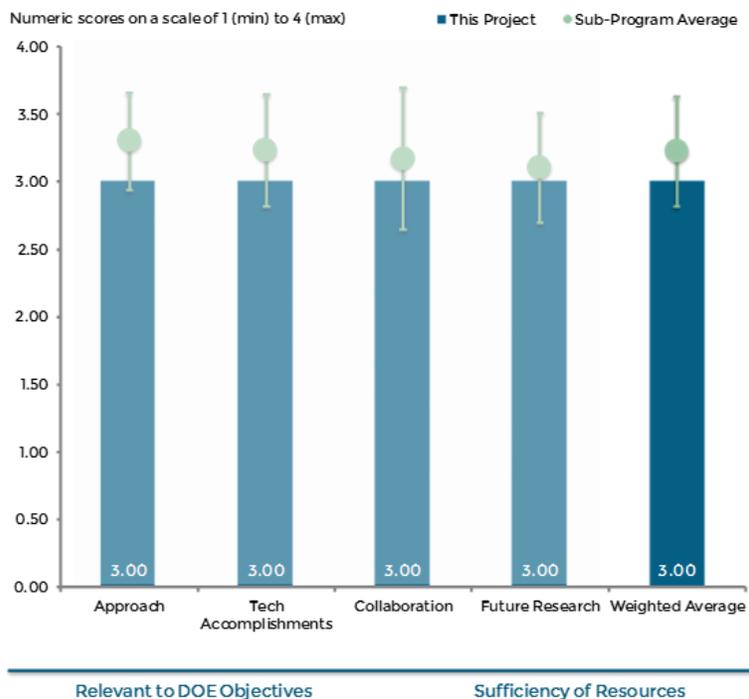
Reviewer 3:

The reviewer stated that the work material is not a pure gradient cathode material but there is a possibility of mismatch between the phases leading to structural failure, and it is not clear about how to improve the performance by using Si/graphite anode. Pre-lithiation is a common approach, but it cannot solve all the problems.

Reviewer 4:

The reviewer commented that the organization of the discussion was difficult to follow, and wondered if the Si section appears to be evaluating Si particle options paired with a variety of carbon materials. The discussion then moved into some level of binder development, but it was not clear which Si carbon matrix had been chosen. The reviewer pointed out that the final structure was shown to have a modestly acceptable short term performance behavior but with a very high first cycle capacity loss, and it is not completely clear what the outcome of all of this was.

The cathode material development appeared to be moving toward the production of gradient designs, but it was not clear how they compared to previous design attempts. The reviewer added there was then some data



es212

Figure 2-30 High-Energy, Long Cycle Life Lithium-Ion Batteries for PHEV Applications: Donghai Wang (Pennsylvania State University) - Electrochemical Energy Storage

presented on proprietary additive addition to the electrolyte for both cathode and anode performance enhancement, but there was no summarization of the results that could provide a reasonable summary.

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 towards DOE goals.

Reviewer 1:

The reviewer observed that the results on the pre-lithiation are very interesting and the work efficiently improves first cycle efficiency. This path should be further investigated, but the cycle stability of the Si anode materials investigated is still not sufficient to meet the target. Moreover, with 500 mAh/g and 3 mAh/cm² the capacity or loading are not outstanding, and thus, it indicates a limited Si amount in the anode for reasons not given. It is recommended to address the potential of the Si-C approach towards higher capacities and the interaction with cycle life.

The reviewer notes that the cathode material investigation of particle size is very interesting, but regarding the dependence on the cooling rate, a theoretical understanding of the experimentally seen effect should be elaborated on. The same is true for the concentration dependence of the lithium zirconate (Li₂ZrO₃) coating. The reviewer questioned why it is optimum at 3%. The high degradation of the material down to 100 mAh/g at C/3 discharge rate after 500 cycles is critical, and the recovery of the capacity at C/20 discharge rate may indicate that connection of particles are lost or have a high resistance, and it is recommended to look in detail on the effect causing this degradation. The reviewer mentioned that the electrolyte and additive work is also very interesting but it is difficult to judge whether one of the alternatives will meet the target of 500 cycles, for the results show only to about 50 cycles. It is recommended to narrow down to one or two candidates for the target cell and extend cycling.

Reviewer 2:

The reviewer stated that the author has made progress and work is in progress for the 250 watt-hour per kilogram (Wh/kg) and 330 Wh/kg batteries but noted that the Li₂ZrO₃ coating is not clearly explained, questioned if it was that done in a batch process, and expressed an interest to know if the process is scalable. For the gradient cathode powders, it will be very important to know how scalable that process is, for the project team mentioned that they have done some scale up experiments. The reviewer added that the authors have produced a variety of powder cathodes and pointed out that, at some point in the project, it will be important to know how reproducible is the synthetic method used for the production of those powders. Similarly, the complicated anode synthesis should be discussed in terms of consistency.

Reviewer 3:

The reviewer expressed that it was difficult to follow the approach and outcomes in a clear way.

Reviewer 4:

The reviewer said that the demonstrated cycle number is still far too low, less than 100, and the understanding and explanation for observed phenomena is not clear.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that the collaboration is well balanced, seems to work effectively, and is well coordinated.

Reviewer 2:

The reviewer expressed that there is good collaboration with other groups and institutions.

Reviewer 3:

The reviewer noted that the collaborators are listed but it was not clear in the data section who was doing what.

Reviewer 4:

The reviewer explained that detailed and specific collaboration activity is missing. All the collaboration starts with the team working, but the what and how are missing.

Question 4: Has the project 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 work is well described and addresses the key issues although it has to be questioned whether all listed open items can be investigated in detail within the short remaining time. The reviewer recommended prioritizing which action items give the highest output in a short time, and the highest benefit to approach the target on cell level.

Reviewer 2:

The reviewer commented that the author should probably down select one or two gradient powders for future studies, and some consideration to scalability of the different processes should be addressed in the future.

Reviewer 3:

The reviewer noted that the future work is a list of many things, but it should be oriented based on prior analysis for it is not just a laundry list.

Reviewer 4:

The reviewer commented this basic work is occurring in a number of the proposals being reviewed at this meeting. The reviewer assumed that a summit meeting specific to this area of development might help determine the most effective pathways to pursue.

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

Reviewer 1:

The reviewer stated that yes, high-energy batteries is what is needed to support the overall objective of petroleum replacement.

Reviewer 2:

The reviewer noted that high-capacity materials are critical to the DOE development pathway.

Reviewer 3:

The reviewer explained that the work is intended to develop a Li-ion battery system with high-energy density, high power density, good cycle life, and safe operation for EV applications, which is essential for the achievement of DOE objectives.

Reviewer 4:

The reviewer pointed out that the work is aimed towards achieving a higher battery energy density necessary to increase the range and market chances for future PHEVs and EVs.

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

Reviewer 1:

The reviewer observed that the project is almost over at this point based on the amount of work reported and the data obtained, and it seems that the resources have been well allocated.

Reviewer 2:

The reviewer noted that a detailed budget plan for individual research efforts is not given.

High Energy Density Lithium-Ion Cells for EV's Based on Novel, High Voltage Cathode Material Systems: Keith Kepler (Farasis) - es213

Presenter

Michael Slater, Farasis.

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 authors are sharply focused in critical areas and are trying different approaches in parallel. Although the ion-exchange approach is adding additional complexity and cost, the authors are aware of it and have planned on tackling the issue with a productive, high-volume operation.

Reviewer 2:

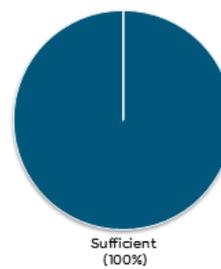
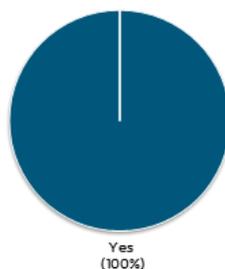
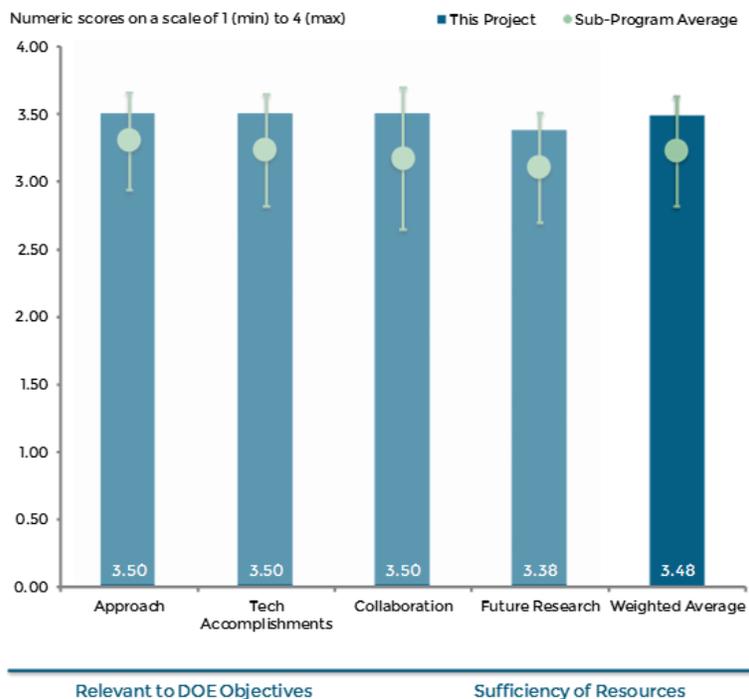
The reviewer affirmed that the proposed approach is comprehensive and promising, but it seems to be focused on energy, where an idea and evaluation for rate performance improvement are also needed. The presentation slides must also be updated from the last year based on new results, as most of the slides are same as the previous one.

Reviewer 3:

The reviewer noted that the project team certainly has a very comprehensive approach that attempts to move every significant component in a cell towards a higher performance. It might be difficult to assess whether each effort is best-of-breed, but still is an ambitious effort.

Reviewer 4:

The reviewer commented that the project team's technical approach is reasonable as where the ion-exchange materials might be a suitable way to reduce the stability problems of the layered-layered material. In particular, it is appreciated that on the cathode material side, both material candidates, layered-layered and Ni-rich NMC, are investigated, which gives the opportunity of a fair comparison and the choice of the better material at the end. The reviewer added that on the anode side, this strategy is not followed, but it is focused on only one development route that has even lower scientific support. That route might be a small weakness.



es213

Figure 2-31 High Energy Density Lithium-Ion Cells for EV's Based on Novel, High Voltage Cathode Material Systems: Keith Kepler (Farasis) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer observed that the amount of work has been significant with the efforts on high-voltage electrolyte, Si containing anodes, evaluation of multiple coatings for the nickel cobalt manganese (NCM) powders used in the Gen-1 cell. The coating approach on NCM powders seems to be very effective.

Reviewer 2:

The reviewer stated that the progress had some very interesting results in a number of technical fronts. Coated cathodes and advanced electrolytes in particular showed interesting improvement options, and the Si anode development follows most of the efforts seen in this year's round of updates, where cycle fade remains an issue and little fundamental understanding about its origins seems to exist.

Reviewer 3:

The reviewer explained that the progress on both cathode material approaches is substantial as also shown in es257 with full cell testing showed reasonable progress and results. Little was reported on the Si-C anode development. It is recommended to intensify the work on this part. In particular, 8% Si content and below 600 mAh/g the cycle life is quite poor and even less acceptable at 1000 mAh/g. The reviewer added that the electrolytes are difficult to judge as there is no information given regarding the changes leading to the improved cycling. Moreover, the target for the high-voltage (HV) electrolyte development is stated to be 4.7 V, but the cycle improvement is only shown at 4.4 V. The reviewer noted that the same is true for the cathode material where capacity measurements were shown at 4.6 or 4.7 V, but the cycling results only at 4.4 V. It is not clear which voltage is needed to meet the targets. The reviewer concluded that it is recommended to harmonize the test condition in the subprojects and set the specifications to the target values.

Reviewer 4:

The reviewer noted that the rate capability must be examined with different C rates.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team has very good collaboration with different groups and institutions.

Reviewer 2:

The reviewer observed that the project team's number of high powered collaborators seem to be working well together, and integrated cell builds with various developed components seems to be moving appropriately.

Reviewer 3:

The reviewer expressed that the project team's collaboration it is well developed and has specific duties for each organization.

Reviewer 4:

The reviewer commented that there are four competent and experienced partners, and the group has the necessary capabilities and the right size to work as a well-coordinated and effective team. On the Si based anode material development, the cooperation could have been strengthened, for example, by an institute providing more detailed analyses or a second material source.

Question 4: Has the project 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 has performed a good effort with good focus on the future goals and execution strategy.

Reviewer 2:

The reviewer observed that the proposed future work is following the initial approach in a suitable and structured way.

Reviewer 3:

The reviewer noted that analysis and evaluation for rate performance and aging must be added.

Reviewer 4:

The reviewer opined that a careful selection of the optimized treatments in each area including anode, cathode, coatings, and electrolytes, is going to be critical, where reproducibility of the results is going to be very important. These are not very standard processes, and even the scale up of the cathode powder should be carefully tested.

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

Reviewer 1:

The reviewer remarked that yes, the project is very relevant for the very important objective of petroleum displacement.

Reviewer 2:

The reviewer concluded that higher energy density cells are a critical component of vehicle electrification.

Reviewer 3:

The reviewer pointed out that the work is aimed towards achieving a higher battery energy density necessary to increase the range and market chances for future PHEVs and EVs.

Reviewer 4:

The reviewer stated that the new cathode and anode electrode materials and Li-ion cell components are required to enable the 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 acknowledged that the project is almost complete and that the resources were well utilized.

Reviewer 2:

The reviewer commented that the project team has a lot of resources, which seem to all be contributing to the project appropriately and effectively.

Reviewer 3:

The reviewer noted that the detailed budget activity is not provided.

First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anodes: Perla Balbuena (Texas A&M University) - es214

Presenter

Perla Balbuena, Texas A&M University.

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:

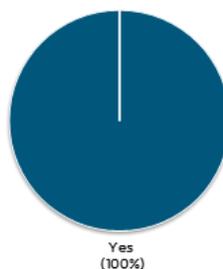
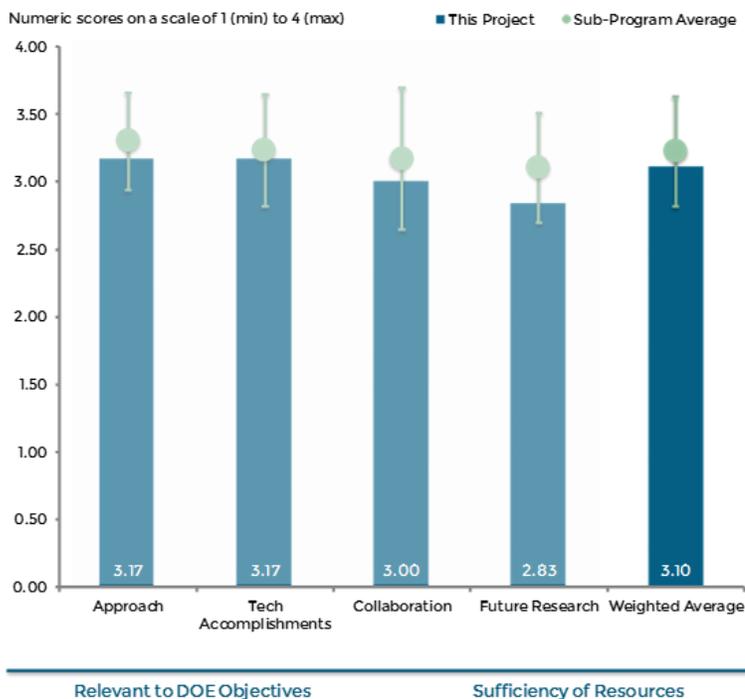
The reviewer explained that this simulation work revealed many details of SEI formation on Si electrodes including lithiated Si, silicon dioxide (SiO₂) covered Si, and ALD coated Si. The approach compliments well with several other Annual Merit Review (AMR) projects.

Reviewer 2:

The reviewer stated that the First Principles quantum mechanical modeling should yield quantitative results and predictions, but the slides for and the Principal Investigator's (PI's) presentation at the AMR were largely qualitative. Furthermore, it was unclear whether any statistical data analysis was performed to ascertain the conclusions based on numerical calculations and simulations. The reviewer added that it was also unclear how sensitive the results are dependent on the initial conditions and configurations. For example, it is hard to believe that the hydroxylated amorphous film, Li_xSiO_{2.48}H_{0.9}, as shown on Slide 7, exists only at this particular composition. The reviewer asked whether the results presented on Slide 8 are statistically significant and independent of initial configurations. Regarding Slide 12, the reviewer asked what "many" refers to in the sentence, "EC/FEC in many cases reduce before LiPF₆." The reviewer inquired about identifying the other cases that also occur and how often. Finally, this reviewer requested clarification on what would be a reasonable agreement as shown on Slide 18, and on what standard deviation the conclusion is based.

Reviewer 3:

The reviewer explained that any Li-ion electrode SEI represents an extremely challenging problem to tackle with calculations of first principles, and the difficulties and benefits associated with the Si electrode makes this work even more challenging and very pertinent. While the reviewer admits not being the best judge of this type of work, the reviewer was impressed with the breadth of the PI's approach. It seemed that the PI is trying to address all aspects of the problem.



es214

Figure 2-32 First Principles Modeling of SEI Formation on Bare and Surface/Additive Modified Silicon Anodes: Perla Balbuena (Texas A&M University) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer observed that the PI has shown many interesting results, but it is difficult to assess the true impact of the PI's calculations and to be sure how to build on the PI's conclusions. The PI also favors the impact of fluorinated ethylene carbonate (FEC) to that of vinylene carbonate (VC), but they have a very different effect on cycling.

Reviewer 2:

The reviewer remarked that progress was made in many areas. The reviewer had two questions. First, the reviewer noted that hydrofluoric Acid (HF) is known to accelerate many degradation reactions. The reviewer asked will HF be formed due to FEC dissociation as fluorine (F) is generated. Second, it is not clear why it is claimed that ethylene carbonate (EC) leads to uncontrolled SEI growth. The reviewer added that, furthermore, more connection with experiments can be made.

Reviewer 3:

The reviewer explained that the first principles of quantum mechanical modeling should yield quantitative results and predictions, but the results presented are qualitative without the support of detailed statistical analysis and sensitivity analysis of initial conditions. The quality of the slides should be improved. For example, there was a grammatical error on Slide 6 and missing horizontal and vertical axis labels on Slide 16.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the PI has a number of collaborations with other modelers and researchers examining the complex material and associated SEI.

Reviewer 2:

The reviewer expressed that more collaboration with SEI property characterization and modeling work will be fruitful to the project team.

Reviewer 3:

The reviewer pointed out that collaborations with experimentalists at University of Rhode Island and NREL have not produced quantitative comparisons between theory and experiments. Also, it is unclear whether the modeling effects have produced quantitative predications to guide experiments.

Question 4: Has the project 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 looks forward to seeing the overall conclusions of this work and the benefits to Si electrode development.

Reviewer 2:

The reviewer observed that because the microscopic models are not sufficiently quantitative and predictive, it is unclear how the microscopic models can be used to effectively develop mesoscopic models.

Reviewer 3:

The reviewer wondered if there are any suggestions on new additives and solvent molecules that should be tested in future work.

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

Reviewer 1:

The reviewer explained that this project will lead to improved high-energy electrode materials, which should reduce costs and enable further electrification of the nation's vehicles and result in improved gas mileage.

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 is effectively using the available funds.

Analysis of Film Formation Chemistry on Silicon Anodes by Advanced In Situ and Operando Vibrational Spectroscopy: G. Somorjai (University of California, Berkeley) - es215

Presenter

G. Somorjai, University of California, Berkeley.

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 praised that the project team has a wonderful approach for attempting to elucidate the composition and structure of SEIs on Si and other surfaces.

Reviewer 2:

The reviewer explained that the PI aims to investigate SEI on the Si surface using in-situ operando (FGVC and Fourier transform infrared spectroscopy (FTIR) in combination with ex-situ X-Ray photoelectron spectroscopy (XPS), scanning electron microscope (SEM) and transmission electron microscope (TEM). This is a powerful but rather common approach, and the use of more advanced complimentary techniques such as time-of-flight secondary ion mass spectrometry (TOF)-(SIMS), depth-profile XPS, and synchrotron spectroscopy, etc., would make the project stronger.

Reviewer 3:

The reviewer stated that the PIs applied in-situ and operando vibrational spectroscopies to directly monitor the composition and structure of electrolyte reduction compounds formed on the Si anodes. The key issue for SEI on Si is the mechanical property and electronic and/or ionic conductivity.

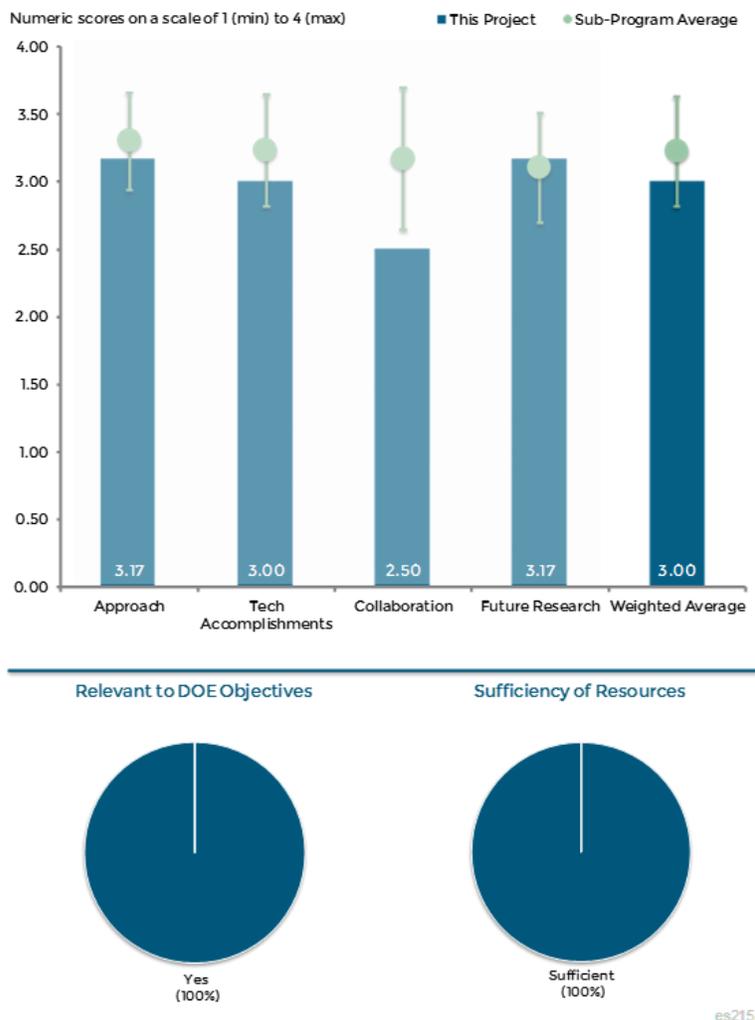


Figure 2-33 Analysis of Film Formation Chemistry on Silicon Anodes by Advanced In Situ and Operando Vibrational Spectroscopy: G. Somorjai (University of California, Berkeley) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer expressed a confusion as to why the fundamental components of the SEI would be different on Si versus on graphite but noted an understanding of why those chemical species would bond differently on Si versus graphite, and perhaps could be different if, say O on Si, contributed to the reaction and resulted in different species being formed. It is excellent that team is investigating the impact of FEC and VC additives on SEI formation, and also impressive that with the time dependence of the SEI layer, the team showing that it grows, and thus, not passivating it for quite a long time.

Reviewer 2:

The reviewer observed that the PIs just tested the SEI composition on Si and graphite, but noted that it was not clear why the composition of SEI on Si is different from the SEI composition on graphite.

Reviewer 3:

The reviewer noticed that the findings of the PI related to VC and FEC are mostly consistent with other researchers in the field and thus, are not uniquely insightful. Other novel claims are on the formation of soluble organic compounds on Si surface such as Li propionate and diethyl 2,5 dioxohexane dicarboxylate versus formation of insoluble compounds on graphite surface, in DEC:EC mixture, which are novel but hard to believe based on prior experience and previous reports. The reviewer added that no experimental evidence was presented during the presentation, whereas in other prior studies, washing Si SEI formed in DEC:EC by DEC or DEC:EC mixtures have been reported not to dissolve the SEI. Thus, claims on the soluble organic components of the SEI are slightly hard to believe because no clear explanation was given on the impact of Si surface on the composition of the organic SEI components.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that a few collaborators have been identified.

Reviewer 2:

The reviewer noted that the PIs did not list the collaborators.

Reviewer 3:

The reviewer remarked that very little information was given on interactions and collaborations with other groups. Given the critical importance of this diagnostics and how many people are interested in the results, it might be valuable to the extent of the collaborations and to some of the many groups trying to use Si in Li-ion cells.

Question 4: Has the project 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 fully supported the continued work on Si surface and the new work on high voltage cathodes. Perhaps collaboration with Kostecki on Mn reactivity in high-voltage cells would be valuable.

Reviewer 2:

The reviewer explained that while some of the future studies could be logical, even without listening to the presentation, the project team was not clearly justified in their talk. Conducting studies to answer many

questions that still remain unclear, in regards to DOE, does not seem to be planned work, for example, why other researchers have not observed soluble SEI on Si, the mechanisms on the SEI differences, etc.

Reviewer 3:

The reviewer said that the PIs failed to provide details on future work.

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

Reviewer 1:

The reviewer said that the investigation of SEI on anodes and cathodes is important for development of EV batteries.

Reviewer 2:

The reviewer stated that gaining a better understanding of the Si SEI may allow one to utilize Si based anodes in the future, which will reduce the cost of Li batteries and contribute to more widespread use of EVs.

Reviewer 3:

The reviewer explained that one of the issues with all of these Si projects (this is not a criticism of this project at all) is that they mainly seem to be working independently of one another. The reviewer would be interested to see a single lead try to integrate the results from this group, from Kostecki, from multiple developers, from universities, etc., into a single coherent picture so that it is clear what answers we have and what questions still need to be attacked. The reviewer suspected that the leading PIs in this field already understand this, but such an effort would probably be extremely valuable to DOE program managers.

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 project funding level is good.

Reviewer 2:

The reviewer mentioned that the PIs have the equipment for the research, and should work with other modelling people and other PIs in the AMR who are working on the same topic.

Optimization of Ion Transport in High-Energy Composite Cathodes: Shirley Meng (University of California, San Diego) - es216

Presenter

Shirley Meng, University of California, San Diego.

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 pointed out that the PI of this project proposed a rather ambitious approach to address essentially almost all critical issues that face the high-energy battery chemistries, which include the capacity and voltage degradation of cathode, and the volume and SEI deterioration of Si. Based on the PI’s knowledge of function point (FP) calculation and spectroscopic characterization tools, the PI designed an encompassing tool suite that was used to also peer into the surface in the bulk of these materials and attempted to establish the work rationales. The reviewer added that these diversified means of spectroscopic and the methodology established in this project will certainly benefit the entire community.

Reviewer 2:

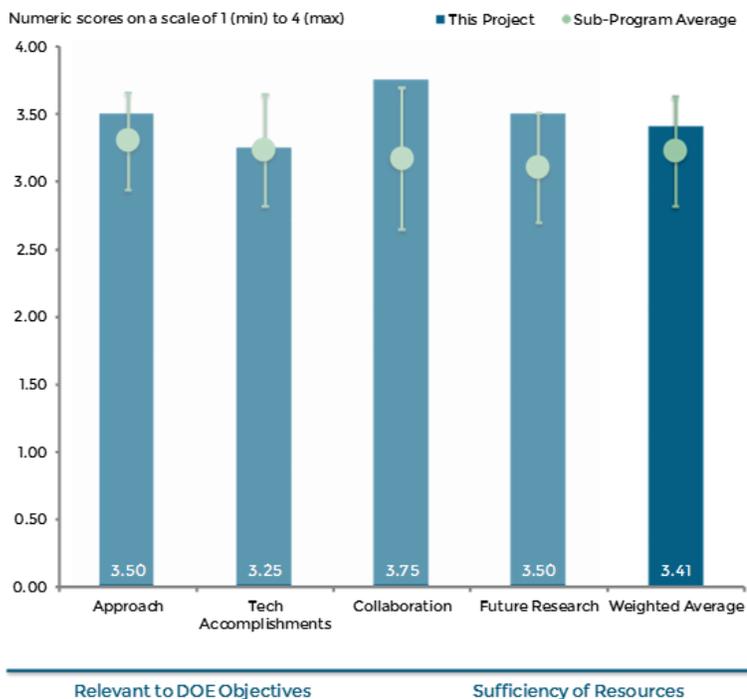
The reviewer observed that like Dr. Grey and Dr. KostECKI, this researcher is focused on the questions and barriers impeding the success of high-energy cells, and brings multiple diagnostics techniques to bear in order to understand the materials and their failure modes.

Reviewer 3:

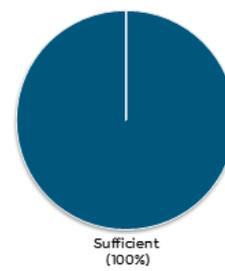
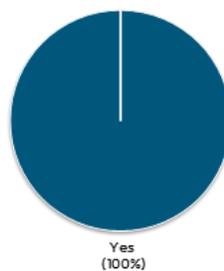
The reviewer stated that the fundamental study on the mechanism for low-voltage stability of high-capacity cathodes and the low first-cycle inefficiency of Si is needed to be addressed.

Reviewer 4:

The reviewer described that the atomistic modeling combined with a scanning transmission electron microscopy (STEM or a-STEM), electron energy loss spectroscopy (EELS), X-ray photoelectron spectroscopy (XPS) and neutron diffraction (ND) were used to understand the dynamic change in the bulk and surface of



Relevant to DOE Objectives Sufficiency of Resources



es216

Figure 2-34 Optimization of Ion Transport in High-Energy Composite Cathodes: Shirley Meng (University of California, San Diego) - Electrochemical Energy Storage

electrodes. The researchers need to elaborate what is unique to their approach compared to other methods, such as X-ray absorption near edge structure (XANES) and extended X-ray absorption fine structure (EXAFS), and the Operando high-resolution transmission electron microscopy (HRTEM), and also need to clarify what knowledge can be obtained with their approach but cannot be acquired with other methods.

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 towards DOE goals.

Reviewer 1:

The reviewer noted that in the second year of this project, the PI has demonstrated a cathode capable of delivering greater than 300 mAh/g with decent cycling stability, where voltage-fading of lithium manganese rich (LMR) was also shown to be mitigated through morphology control rather than surface coating; however, the 80 cycle is still not convincing enough to claim to be effective, although the results are encouraging. The section of SEI chemical composition on the Si anode is less impressive than the cathode work, as similar results have been described in literature a few years back, but the newly established methodology is expected to reveal new perspectives. The reviewer added that the use of neutron characterization is especially innovative, which differentiates the distribution of Li from Li-layer and TM-layer, and thus, will help further understand why the Li-excess cathode material fades in long-term cycling and provide guidelines for designing future materials. This reviewer expressed that more new info will become available if the PI continues to exploit this technique, and perhaps, an improvement in pouch cell design could help.

Reviewer 2:

The reviewer stated that the accomplishments include a large number of excellent results, but expressed the need to point out that the voltage stabilization claimed on Slide 7 looks highly doubtful. The voltage on charge increases on the curve on the right, meaning that the voltage change is at least partly the result of impedance rise, and thus, must be removed from the data to understand the true voltage decay with cycling. The reviewer added that it would also be valuable to understand why this researcher thinks that surface modification is impacting voltage fade when ANL's exhaustive study last year found that it did not. The reviewer mentioned that the cathode SEI work was impressive.

Reviewer 3:

The reviewer expressed the need to clarify the mechanism of why the surface modification can improve the voltage stability. The reviewer asked how does the lithiation/delithiation mechanism of high-capacity cathode obtained from Operando neutron relate to the voltage decay. The reviewer asked why the thick SEI formed on Si from FEC-electrolyte has a more stable cycle life. The mechanical property of SEI may be more important for Si.

Reviewer 4:

The reviewer explained that the Li-ion de-intercalation activities of Li-excess were investigated by the Operando neutron scattering technique. The solid-electrolyte interphase, or SEI, composition in Si-based anode materials was measured, and the fluoroethylene carbonate, or FEC, co-solvent and other additives were found to promote the formation of a stable SEI. The reviewer expressed that the research team needs to clarify what new insight into the cathode evolution mechanism can be provided based on the characterization results, and added that it would be great if the research team can identify the critical factors that govern the formation of SEI.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer commented that the number and breadth of the collaborators is impressive and excellent which includes universities, national laboratories, and battery developers, and that the Si SEI results are excellent. The reviewer encouraged someone to review and integrate the multiple findings on this critical topic and to communicate an overall understanding of current SOA and what is known.

Reviewer 2:

The reviewer pointed out that the PI showed an excellent record of collaboration and coordination with other institutions.

Reviewer 3:

The reviewer stated that the PI has built a nationwide network to perform the collaborative research.

Reviewer 4:

The reviewer noted that the PI has collaborated with several groups on the Battery Materials Research (BMR) team.

Question 4: Has the project 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 remarked that it is excellent that the PI is focusing on the impact of FEC on the Si SEI.

Reviewer 2:

The reviewer said that the objective proposed for future research is aligned very well with what DOE is focusing on.

Reviewer 3:

The reviewer noted that the PI plans to study the chemical stability of SEI upon cycling, but asked about any plans to study the mechanical property of SEI.

Reviewer 4:

The reviewer observed that several important issues will be addressed in the future, but suggested that the future work to be focused on the evolution of the interface between the electrode and the electrolyte, where an emphasis is placed on the clarifying the underlying mechanism of SEI and on identifying the critical factors that govern the formation of SEI. Furthermore, the reviewer commented that the rationale for developing the strategy for prevention of SEI formation should be addressed.

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

Reviewer 1:

The reviewer stated that the ongoing research is well aligned with the mission and the objective of the DOE program.

Reviewer 2:

The reviewer noted that this project supports the DOE objective.

Reviewer 3:

The reviewer stated that yes, the project supports the DOE objective for obvious reasons.

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 sufficient for the work, but would support further funding if it were requested.

Reviewer 2:

The reviewer noted that the resources are sufficient.

Reviewer 3:

The reviewer mentioned that the PI should also add modelling components to explain the results.

Daikin Advanced Lithium-Ion Battery Technology - High-voltage Electrolyte: Ron Hendershot (Daikin America) - es217

Presenter

Joe Sunstrom, Daikin America.

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 noted that the proposed fluorocarbon (FC) electrolyte should be effective in improving the cycle life at 4.6 V and in improving the safety performance.

Reviewer 2:

The reviewer commented that it seems that the authors have been working in areas that are critical to the objective of the program, and at some point, it should be of interest to compare the data obtained with Li NCM 111 (1/3, 1/3, 1/3) with a cathode containing higher Ni content. In the future it will be important to better understand the mechanism involved with the increased gassing as the FEC content is increased.

Reviewer 3:

The reviewer described that the PI adopted a typical industrial research and development (R&D) approach for new product development from benchmarking, selection and optimization. However, without details of the process, it is hard for the reviewer to further comment on the matter.

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 towards DOE goals.

Reviewer 1:

The reviewer described that the PI demonstrated the significant improvements of FC electrolyte composition that out-perform the traditional hydrocarbon electrolyte at high-voltage cells. Such improvements included cycle-ability and safety. The reviewer also noted that the milestones were all reached.

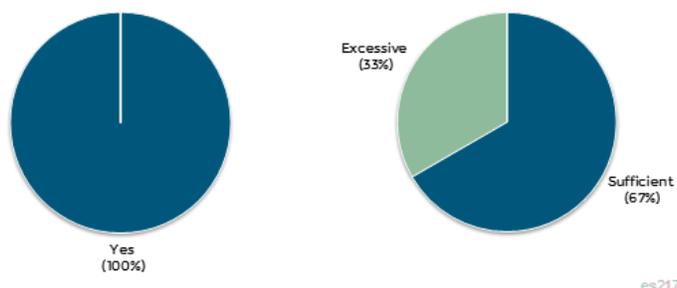
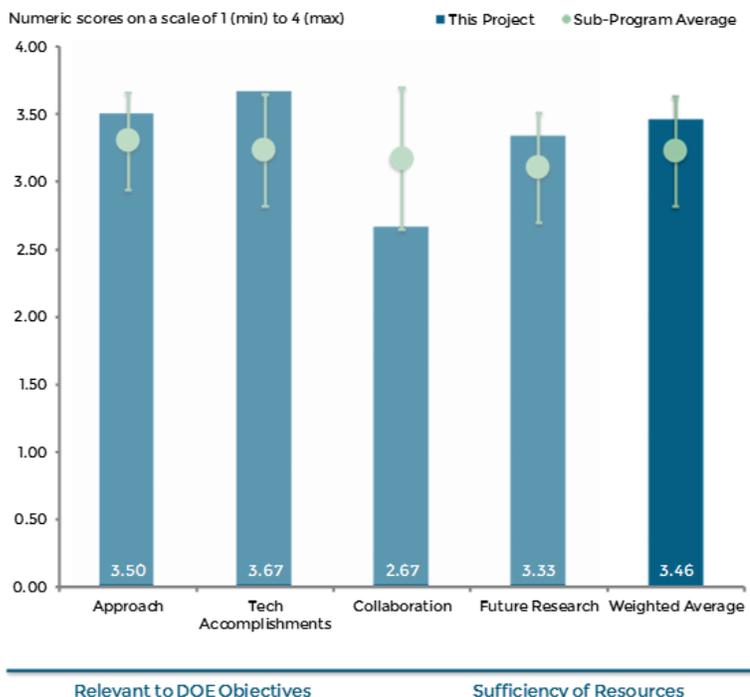


Figure 2-35 Daikin Advanced Lithium-Ion Battery Technology - High-voltage Electrolyte: Ron Hendershot (Daikin America) - Electrochemical Energy Storage

Reviewer 2:

The reviewer commented that seems that the authors are on the right track for this month, the team is demonstrating stable cell performance at 4.6 V, and last January, the authors delivered 10 interim cells to DOE.

Reviewer 3:

The reviewer stated that the FC electrolyte was shown to be effective in improving the cycle life, especially at elevated temperatures. The FC electrolyte also improved the overcharge safety performance. However, it was not clear why the FC electrolyte was not effective in improving the calendar life at 4.6 V. The reviewer added that the FEC additive was demonstrated to be effective on anodes such as Si, and thus, it was not clear how FEC also provided enhancement for the high-voltage cathode and electrolyte interface.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that the extent of collaboration with Coulometrics was not clear.

Reviewer 2:

The reviewer commented that the team's collaboration could be improved. The authors mentioned that in the last part of the project, which involve surface characterization, will be pursued outside the company.

Reviewer 3:

The reviewer stated that the PI still lacks collaboration with other institutions, although the project team realized the significance of the matter.

Question 4: Has the project 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 is well described and reasonable. The PIs should extend the fundamental understanding of the FC electrolyte and preferably collaborate with either national laboratories or universities.

Reviewer 2:

The reviewer commented that some consideration should be given to the scalability of the process discussed, and in particular, to the synthetic work related to the electrolytes.

Reviewer 3:

The reviewer remarked that the project team needs to propose some future effort to de-conflict the results between cycle life versus calendar life gassing results, and should also propose effort to understand how FEC enhanced high-voltage cathode. The insight from understanding the mechanism will help to discover other additives for high-voltage cathodes.

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

Reviewer 1:

The reviewer commented that developing an electrolyte that can work at high-voltage effectively and safely is relevant to the goal of developing high-energy density batteries for EVs.

Reviewer 2:

The reviewer said that yes, electrolytes for high-voltage applications are badly needed for high-energy density cells.

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

Reviewer 1:

The reviewer pointed out that the PI has adequate resources for the proposed research and is achieving the milestone and goals.

Reviewer 2:

The reviewer noted that the project is finishing this year and it seems that the authors have produced a reasonable amount of data based on the funding.

Fluorinated Electrolyte for 5 V Lithium-Ion Chemistry: John Zhang (Argonne National Laboratory) - es218

Presenter

John Zhang, Argonne National Laboratory.

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 work effort has been much focused on the barriers and imagines that the synthetic efforts are not easy, but has a very nice contribution from the theoretical area.

Reviewer 2:

The reviewer said that the PIs try to synthesize fluorinated electrolyte guided by theoretical calculation. Although the approach of using the highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital (LUMO) only is over-simplified, it is a good starting point, and the chemical synthesis is the strong point of approach.

Reviewer 3:

The reviewer observed that the approach is similar to that in 2014 where the project team proposed to expand the electrochemical window by introducing cathode additive and new solvents. These general approaches should be effective to mitigate the low electrolyte oxidation barrier, cycle life barrier, high- and low-temperature barrier, and the safety barrier.

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 towards DOE goals.

Reviewer 1:

The reviewer noted that the progress is sharply focused on the critical areas. At some point in the future, the authors should focus also in how scalable some of the synthetic efforts are.

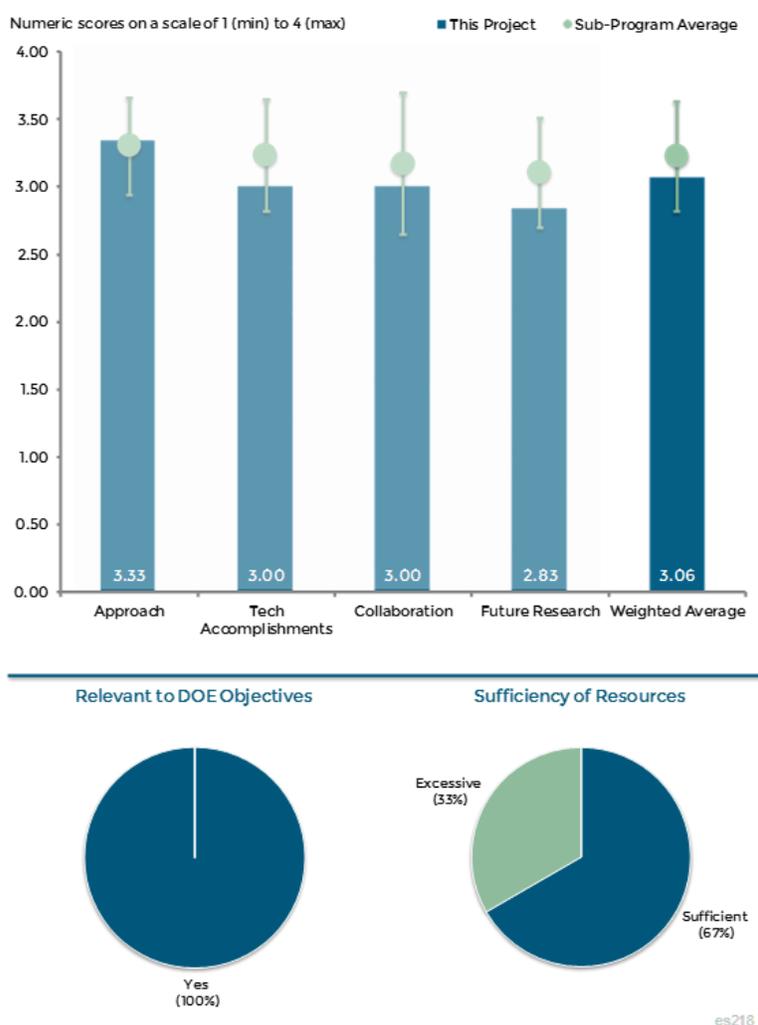


Figure 2-36 Fluorinated Electrolyte for 5 V Lithium-Ion Chemistry: John Zhang (Argonne National Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer explained that various fluorinated electrolytes were synthesized and tested in the cells. Even though the chemical synthesis was the bright side of the project, the technical accomplishments on the characterization were weak, especially, for example, the in-depth understanding of the electrolyte working in a cell interaction with electrodes. The reviewer added that it is interesting that most of the peer-reviewed publication was co-authored with a senior researcher who is not on the team, and also realized that the PI did not include the response to the reviewer's comments from last year.

Reviewer 3:

The reviewer stated that in the ANL section of the presentation, most of the slides seemed to be similar to that of 2014, where most of the cycle life improvement data was based on only single-cell and 50-100 cycles. To be impactful, the project team needs to show cycle life based on multiple cells and at least 300 cycles on the optimized electrolyte. The reviewer added that in order to demonstrate that the electrolyte will meet PHEV or EV needs, the team needs to demonstrate that their electrolytes improve high-temperature stability without compromising low-temperature performance. There is limited performance data from additives from the synthesis of which was presented in 2014, and thus, the reviewer expressed an expectation to see more performance data in 2015, for the team needs to link the chosen additives to their proposed approach rationale. The reviewer expressed, for example, if the room temperature (RT) and 55°C cycle life improvement from FEC, TF-PC3 and lithium difluoro-oxalato-borate (LiDFOB) additives be attributed to the cathode/electrolyte interface, and if so, how these additives improved the cathode and electrolyte interface. There is lack of continuity from the 2014 effort. The reviewer also expressed if there is the follow-up on the good results of the E3, E4, E5, E6 and high voltage electrolyte-1 (HVE1) electrolytes presented in 2014, and if there a synergistic effect to combine the aforementioned additives with high voltage electrolyte-3 (HVE3).

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

The reviewer stated that there seems to be strong collaboration. The marriage between theory and organic synthesis is very interesting. The data related with the non-flammable fluorinated electrolyte was impressive.

Reviewer 2:

The reviewer stated that the PI and co-PI of the U.S. Army Research Laboratory (ARL) demonstrated close collaboration, but the collaboration with others were not evident.

Reviewer 3:

The reviewer observed good collaboration with ARL. The extent of collaboration with the other performers was not clear.

Question 4: Has the project 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 pointed out that the project is finishing this year, and that the electrode surface analysis can prove to be important. The authors should probably try to down select the synthetic work that has higher chances of success going forward, and that the synthetic efforts in research and development should also, at some point, be related to some practical considerations such as scalability.

Reviewer 2:

The reviewer noted that the proposed future research is reasonable, but should include a more fundamental understanding of the work.

Reviewer 3:

The reviewer stated that the project team needs to propose some future effort to address the low-temperature performance without sacrificing performance at high temperatures. The team also needs to propose a future effort to improve calendar life and to give a rationale on why the team proposed to pursue the sulfone-based electrolyte. It was not clear why the team did not propose to combine the fluorinated solvents with the additives for future effort.

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

Reviewer 1:

The reviewer remarked that yes, more stable electrolytes for high-voltage and less flammable applications are critical for the development of high-energy batteries.

Reviewer 2:

The reviewer noted that the proposed research is relevant to the DOE goal for high-energy Li-ion battery 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 observed that the project is reaching completion this year. The authors have put together a tremendous synthetic effort, and thus, the resources were well invested.

Reviewer 2:

The reviewer noted that the PIs have access of more than adequate resources for the research.

Novel Non-Carbonate Based Electrolytes for Silicon Anodes: Dee Strand (Wildcat Discovery) - es219

Presenter

Dee Strand, Wildcat Discovery.

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 approach is very focused on the development of non-carbonate electrolyte for the Si alloy anode, which is a very complex problem because as the standard electrolyte is replaced, new additives and salts have to be developed.

Reviewer 2:

The reviewer stated that the PI used high throughput techniques to screen large amount of non-carbonate electrolytes for Si anode. Although such an approach is effective for fast screening, the PI should either engage fundamental research so the screening can be more focused, or develop a feasible statistical method to analyze the large amount of data points.

Reviewer 3:

The reviewer explained that Si-stable additives and non-carbonate solvents were proposed for an optimized electrolyte that is stable with Si anode, and expressed that is not clear how non-carbonate solvents combined with the additive will form more stable SEI than carbonate solvents combined with the additive. The project team needs to provide their rationale for selecting the non-carbonate solvents that are stable with Si alloy anode, and the additives that will form SEI in the absence of EC.

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 towards DOE goals.

Reviewer 1:

The reviewer reported that it seems that the authors have accomplished greater than 200 cycles to 80% capacity with non-carbonate formulations, but could be of great interest to know if 500 cycles are finally achieved. At

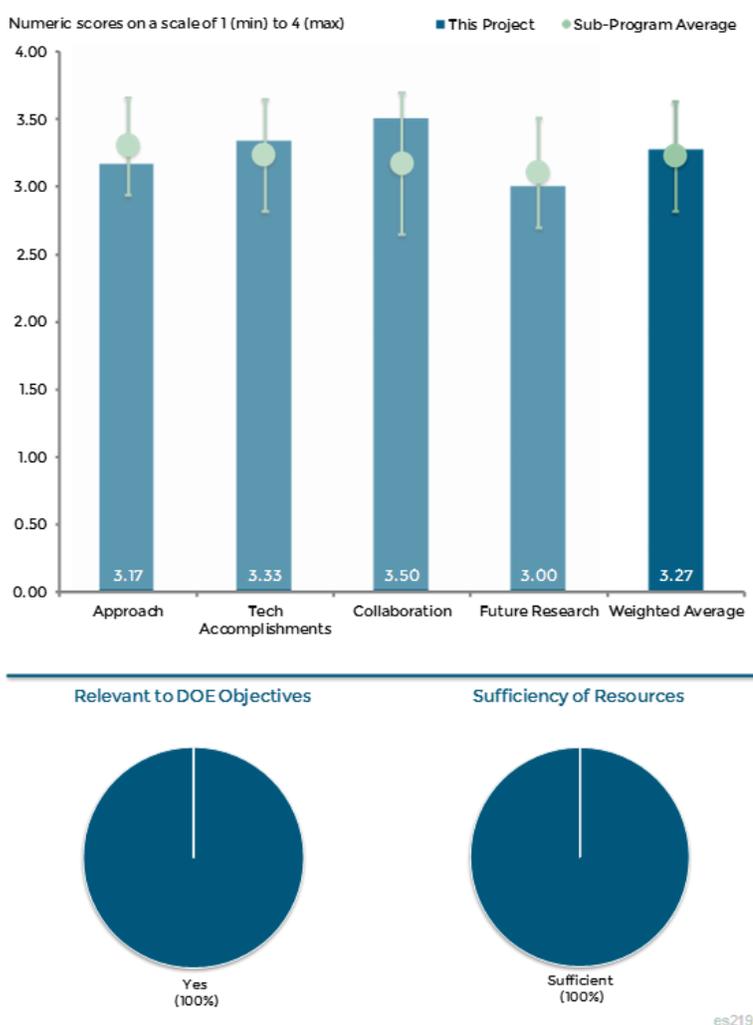


Figure 2-37 Novel Non-Carbonate Based Electrolytes for Silicon Anodes: Dee Strand (Wildcat Discovery) - Electrochemical Energy Storage

some point, the authors should give more detail about the type of NMC cathode that the team is using. The reviewer added that ideally, the electrolyte should be stable towards a variety of cathode powders.

Reviewer 2:

The reviewer observed that the milestones were achieved. Although a large amount of electrolytes were tested, the reviewer questioned the statistical significance of the results, for example, how reliable the conclusion is and what the team's confidence level is.

Reviewer 3:

The reviewer commented that there was not much meaningful data presented that allow the progress to be assessed, where the most significant data presented was the specific capacity verses cycle number plot. There was no data on rate capability, voltage stability window, and initial irreversible capacity loss of the optimized electrolyte in a NMC/Si cell. The reviewer added that in the absence of this data, it is difficult to assess if the team's optimized electrolyte will improve the energy density of a Li-ion cell based on Si alloy anode, especially when the team attributed the low-capacity in 18650 cells to a non-optimized design.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team seems to have very good collaboration with 3M Company and ANL.

Reviewer 2:

The reviewer noted that the PI collaborates with many other institutions indeed.

Reviewer 3:

The reviewer said that the project team has adequate collaboration with ANL and 3M Company, though it was not clear the extent of data sharing.

Question 4: Has the project 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 additional testing on other Si sources is recommended as already mentioned by the authors, where high-voltage stability and large cell format were already mentioned.

Reviewer 2:

The reviewer noted that the statistical approach should be added to the future research.

Reviewer 3:

The reviewer said that the proposed future work was very vague. The project is only 68% completed, and thus, the project team should be more specific on what future work and why, for example, what additives combinations and why.

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

Reviewer 1:

The reviewer remarked that yes, the project is very relevant to petroleum displacement. High-capacity Si anodes is one of the areas that can increase the energy density of a battery.

Reviewer 2:

The reviewer said that the development of non-carbonate electrolyte for Si anode is relevant to the goal of developing high-energy density 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 observed that the project is finishing this year and that the authors got a lot of work done with the resources allocated.

Predicting Microstructure and Performance for Optimal Cell Fabrication: Dean Wheeler (Brigham Young University) - es220

Presenter

Dean Wheeler, Brigham Young University.

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 ability to detect localized changes in the conductivity of an electrode is incredibly valuable, and that this work is moving in the right direction to accomplish this goal. Battery failure begins with localized failure where identifying and eliminating these failures will lead to longer cycle lives, the use of potentially higher currents, and also an improvement to their manufacturing.

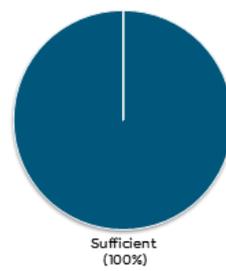
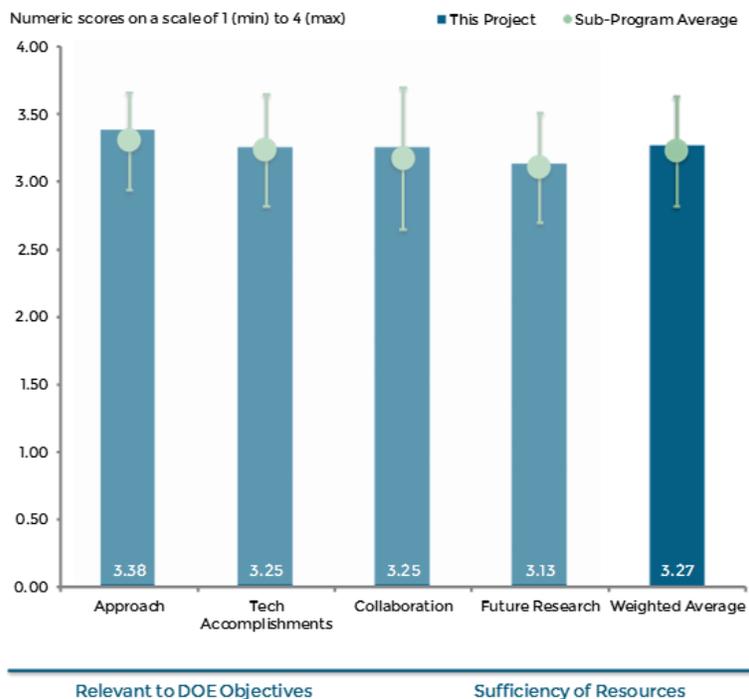
The reviewer expressed a curiosity about the expected implementation of this technology as an on-line process monitoring tool.

Reviewer 2:

The reviewer noted that it is a good approach to test the microstructure and performance for optimal cell fabrication.

Reviewer 3:

The reviewer described that this approach is primarily a two-part effort. The electrode conductivity measurement studies were initiated first with a unique and excellent approach this year where the prediction of the electrode microstructure from the slurry is a much more difficult problem and was initiated in a significant way. The approach on this effort is also unique, but somewhat surprising. The reviewer expressed an expectation that the slurry drying problem would be addressed through some volume-averaged continuum-based heat and mass-transfer and surface-tension model. Alternatively, a more complex model could be used that specifically tracked the interactions of the individual particles and the solvent and binder liquid. The reviewer pointed that either of these approaches would have been very challenging, but the PI was very innovative in that the utility of an existing molecular dynamics program to describe the slurry drying process and resulting electrode morphology was identified.



es220

Figure 2-38 Predicting Microstructure and Performance for Optimal Cell Fabrication: Dean Wheeler (Brigham Young University) - Electrochemical Energy Storage

The reviewer expressed that it seems that the PI has sacrificed the long term predictive capability for a short term progress. The model being developed relies on particle interaction functions that are somewhat unique to each slurry. The reviewer added that it is not clear how the PI relates these functions to things one can measure like surface tension properties. The PI appears to be generating a model that will be most useful for correlating results.

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 towards DOE goals.

Reviewer 1:

The reviewer commented that the PI has made excellent progress towards the project's goals on both aspects of the work, for during last year's review, the reviewer questioned the PI's ability to quickly develop a model for the slurry drying process. As described above, the PI has found an innovative way to do accomplish that task.

Reviewer 2:

The reviewer explained that up to this point, the research team has constructed a test set-up for each electrical and ionic conductivity. The work with the former team was largely completed by the last year's review, but the ionic conductivity testing has shown strong progress at this point in the work. The reviewer pointed out that the experimental set-up is still being refined, as well as the model, and although both are imperfect, given the preliminary stage of this effort, the current status is admirable. The reviewer added that it is good that the team continues to seek out additional samples, but it remains critical that this model is not limited to a specific material. Additionally, because the model seems to use a high percent of inactive material, the reviewer expressed to be not sure of the impact of this observation.

Reviewer 3:

The reviewer noted that more experiments are recommended to perform with standard commercial electrodes to demonstrate their feasibility.

Reviewer 4:

The reviewer stated that the project team designed, fabricated and tech-transferred the first generation surface conductivity probe, and this model also seemed to show good correlation between measured and predicted electrode fabrication properties. However, it is unclear if the probe will have sufficient length scale resolution of millimeter (mm) or smaller, to detect the electrode. It is also unclear if the probe will have fast response time to measure the conductivity in real time in a mass production environment. In order to demonstrate the impact of the dynamic particle-packing (DPP) model, the project team needs to use the DPP model to guide the slurry parameters, for example, viscosity and shear speed. The reviewer added that the project team also needs to correlate the optimized slurry parameters to the electrode with more uniform conductivity, and ultimately, to validate this modeled electrode with the actual performance gain in cells.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer commented that the team is actively working with industrial and laboratory partners to commercialize this technology, and are also actively working on technology transfer, which is exceptional. The reviewer stresses broader engagement, but finds no fault to be found with the current efforts and reasonably expects future efforts to attract new partners.

Reviewer 2:

The reviewer said that the PI has generated significant collaboration with industry, other program participants, and the national laboratories.

Reviewer 3:

The reviewer noted that the project team has good collaboration and interaction.

Reviewer 4:

The reviewer said that the project team has good collaboration with national laboratories and A123, but collaboration should also include making cells to validate the team's modeled electrode.

Question 4: Has the project 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 overall, the PI has a very good forward plan, and it will be interesting to see the adequacy of his model in achieving the PI's goals.

Reviewer 2:

The reviewer commented that the team is focused on increasing instrument measurement reliability and developing new probes to more fully characterize conductivity. The work on the model is ongoing in order to get better agreement with experimental data. The reviewer said that it will be interesting to track this progress at future AMRs. More specifics on the barriers of the model that are being addressed would have been desirable.

Reviewer 3:

The reviewer explained that in order to have impact, it is important for the project team to demonstrate better performance, for example, higher utilization, in a practical cell, for example, 18650 or pouch cell, with an optimized electrode based on the DPP model.

Reviewer 4:

The reviewer noted that the proposed future work should include testing of various commercial electrodes.

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

Reviewer 1:

The reviewer said that this project will lead to more optimized electrode microstructures, that both improve the energy efficiency and the cycle life of batteries. Ultimately, this work will lead to reduced battery costs enabling further electrification of the nation's vehicles and improved gas mileage.

Reviewer 2:

The reviewer noted that this project work will reduce petroleum use.

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

Reviewer 1:

The reviewer mentioned that the researchers are performing admirable work with the resources provided. Milestones and go or no-go decision points are being hit as would be expected.

Reviewer 2:

The reviewer stated that the PI has effectively chosen a path, in such a way, to accomplish the project's goals and overcome its barriers within the PI's budget.

A Combined Experimental and Modeling Approach for the Design of High Coulombic Efficiency Si Electrodes:
 Xingcheng Xiao (General Motors)
 - es221

Presenter

Xingcheng Xiao, General Motors.

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 observed that the project team has a reasonable approach which used modeling to guide experimental design of artificial stable SEIs for Si anode.

Reviewer 2:

The reviewer said that this project addresses Si-based electrodes limitation by conducting research on the understanding and design of a stabilized nano-structured Si anode to improve Li-ion battery capacity.

Reviewer 3:

The reviewer stated that ALD coating definitely improves the stability of the Si anode and more experiments are needed rather than just performing computation.

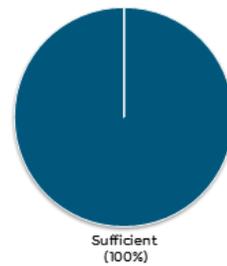
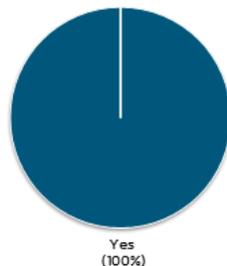
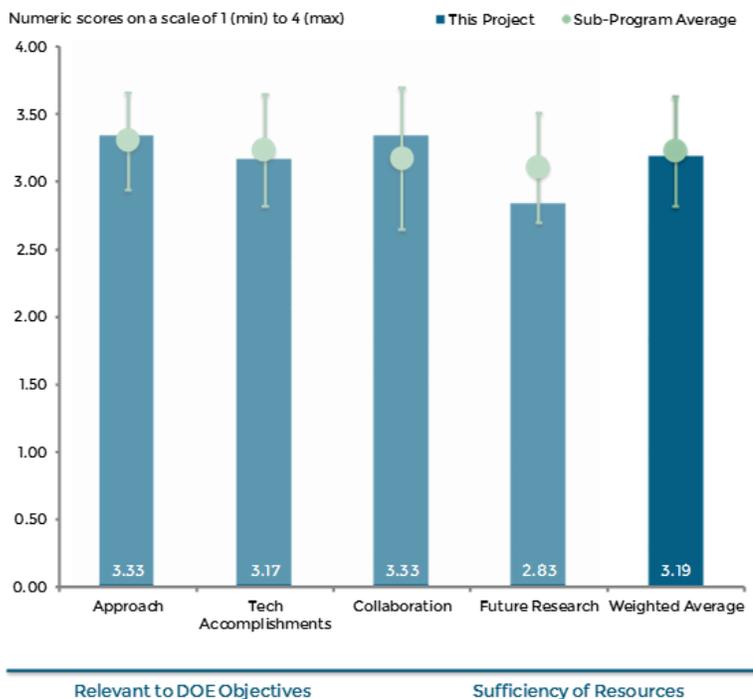
Question 2: Technical Accomplishments and Progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

Reviewer 1:

The reviewer stated that the technical progress that has been made so far is impressive. However, it is unclear if the milestone of comparing the modeling results of SEI deformation and stability with in situ multi beam optical stress sensor (MOSS) measurement has completed or not.

Reviewer 2:

The reviewer explained that the combined DFT and continuum model has been developed to predict the mechanically stable Si-C core-shell structures, which stabilize the SEI layer and accommodate the volume



es221

Figure 2-39 A Combined Experimental and Modeling Approach for the Design of High Coulombic Efficiency Si Electrodes: Xingcheng Xiao (General Motors) - Electrochemical Energy Storage

expansion of Si. However, how the Si-C yolk stability is better than the Si-C core shell structure, needs to be explained.

Reviewer 3:

The reviewer reported that there seemed to be a disconnect between the modeling and experimental data, for there was no experimental cycling data on the beneficial effect of artificial SEI from ALD coating that was predicted by modeling. The project team devoted lots of effort on understanding and modeling of the SEI, but good cycling results were obtained from architecture design of Si particles such as graphene encapsulation and the York-Shell encapsulation. The reviewer expressed that the team needed to demonstrate a good cycle life with 3.5 mAh/cm² loading based on the approximately 1,000 mAh/g reversible capacity, and not based on the 2,865 mAh/g of initial capacity.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the PIs have good collaborations with other institutions.

Reviewer 2:

The reviewer commented that the project team has good collaboration with other national laboratories and University of Waterloo.

Reviewer 3:

The reviewer noted that the project team has good collaboration.

Question 4: Has the project 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 Li-ion battery for vehicle applications typically experience variety of charge-discharge rates, and suggested to add the understanding and characterization of designed coating to see if it is stable at higher charge and discharge rates and different temperatures.

Reviewer 2:

The reviewer noted that more experiments are recommended rather than computation work.

Reviewer 3:

The reviewer explained that the project team's data showed that the yolk-shell Si/C had better cycle life than the core-shell Si/C, but it was not clear why the team chose to focus on the core-shell Si/C for future work. In addition, the team should apply ALD coating on the yolk-shell Si/C to see if there is additional improvement. The reviewer added that the team claimed that mechanically stable coating on Si can be achieved based on the identified the proper coating thickness based on the selected coating material as shown on Slide 15, and the team needs to propose an effort to validate this claim in cells.

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

Reviewer 1:

The reviewer said that the project supports the overall DOE objectives as it makes efforts to improve Si based anode's performance and life for Li-ion applications.

Reviewer 2:

The reviewer noted 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:

The reviewer observed that it appears that there are sufficient resources for this project to achieve the proposed goals as planned.

Electrode Architecture- Assembly of Battery Materials and Electrodes: Karim Zaghib (Hydro Quebec) - es222

Presenter

Karim Zaghib, Hydro Quebec.

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 of this project is address the Si electrode's poor life issue through the electrode architecture design, and that it is a good approach.

Reviewer 2:

The reviewer stated that the approach essentially takes a somewhat unique method of producing uniform micro-Si powder and characterizing this material as an electrode structure. This is an interesting method, and perhaps has a role in the production of Si for anode materials. The reviewer added that the basic improvement in understanding of the issues associated with Si anode development is not as strong, as referred to most of the Si based materials development activities on the agenda, but is not a negative on a relative basis to other programs.

Reviewer 3:

The reviewer commented that the project team has done excellent work on methods of producing electrode materials, but not enough strategy and focus on electrode design. The composition of the electrode, for example Si content, should be clearly stated to allow for data interpretation.

Reviewer 4:

The reviewer explained that the high-risk, multi-step process for development of nano-silicon anode material leads to very high-energy batteries, but that significant cost reduction is needed for nano-silicon anode technology to be practical.

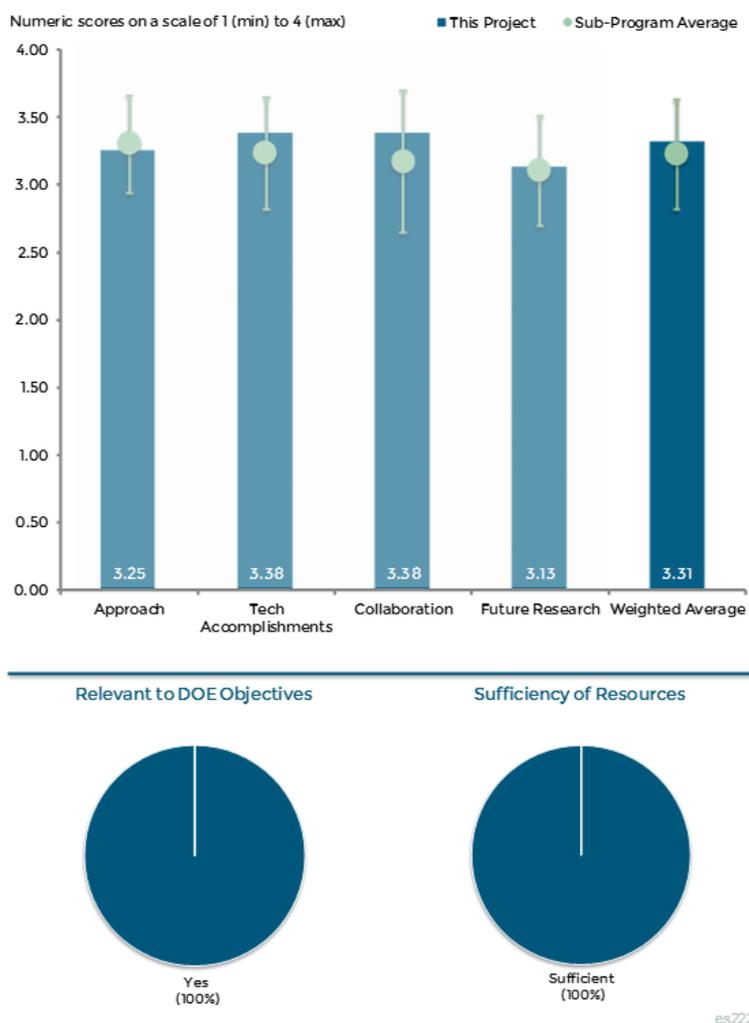


Figure 2-40 Electrode Architecture-Assembly of Battery Materials and Electrodes: Karim Zaghib (Hydro Quebec) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer remarked that at the very least, it was impressive to see some encouraging data on electrode structures that had very high percentages of Si, which is perhaps a good material to feed into other novel electrode architectures.

Reviewer 2:

The reviewer stated that the technical achievement in this project is good, as Si nano-powder was produced and evaluated in cell. In-situ TEM analysis for Si nano-powder was conducted and samples were delivered to collaborators for their projects.

Reviewer 3:

The reviewer explained that the technical accomplishments transitioned rapidly to full-size high-performance cells, which is impressive. More full-size cells need to be subjected for extensive testing for performance and life in accordance with DOE, United States Advanced Battery Consortium (USABC) Systems, and Society of Automotive Engineers (SAE) standard test procedures, however, USABC Systems' cost model needs to be completed for this technology.

Reviewer 4:

The reviewer commented that the project team needs a clear strategy for the electrode design, which is one the main objectives of this project, and that it is important to get a better understanding of the gassing issue at every step of the process, including during electrochemical testing.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer mentioned that the project team had good collaboration with partners in several areas. The overall Hydro Quebec' (HQ) team performance and capabilities are very strong from earlier programs in advanced batteries.

Reviewer 2:

The reviewer noted that the project has a strong and highly respected team.

Reviewer 3:

The reviewer stated that project team's collaboration seemed to revolve around the delivery of materials to other organizations, where it would be interesting to have gotten some results from these collaborators.

Question 4: Has the project 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 it will be interesting if the effect of working tempering on the relationship of life and cycle number will be included in the future study.

Reviewer 2:

The reviewer commented that the continued R&D needed to have lower costs for materials processes, and that demonstration of full capability of this technology has to be done with independent testing at DOE laboratories.

Reviewer 3:

The reviewer explained that the activities should be prioritized to support the project objectives. HQ's desire to become a provider of baseline electrode materials should be outside of the program. The reviewer added that the comparison of the results generated by the partners will be very important.

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

Reviewer 1:

The reviewer noted that the project has a strong and highly respected team.

Reviewer 2:

The reviewer explained that this technology can significantly improve EV and PHEV performance, life, and cost, and has potential to significantly improve vehicle range and market penetration.

Reviewer 3:

The reviewer stated that this project supports the DOE objectives by studying Si nano-powder and provides samples to support other projects.

Reviewer 4:

The reviewer that success of this project will enable next generation EV batteries.

Reviewer 5:

The reviewer noted that Si is a major material on the roadmap to high-capacity cells.

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 project resources should be devoted to a more complete detailing of cell tests results for performance and life, and that additional funding may be required to support this work.

Reviewer 2:

The reviewer commented that sufficient and more focus will help in achieving the project objectives.

Hierarchical Assembly of Inorganic/Organic Hybrid Si Negative Electrodes: Gao Liu (Lawrence Berkeley National Laboratory) - es223

Presenter

Gao Liu, Lawrence Berkeley National Laboratory.

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 the use of conducting polymer for Si anode is an excellent approach.

Reviewer 2:

The reviewer commented that the project team has a novel approach of using conductive polymer binder to mitigate the Si expansion issue and to improve energy density.

Reviewer 3:

The reviewer said that the PI developed a unique approach to address the short life for Si based anode.

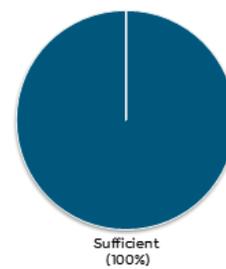
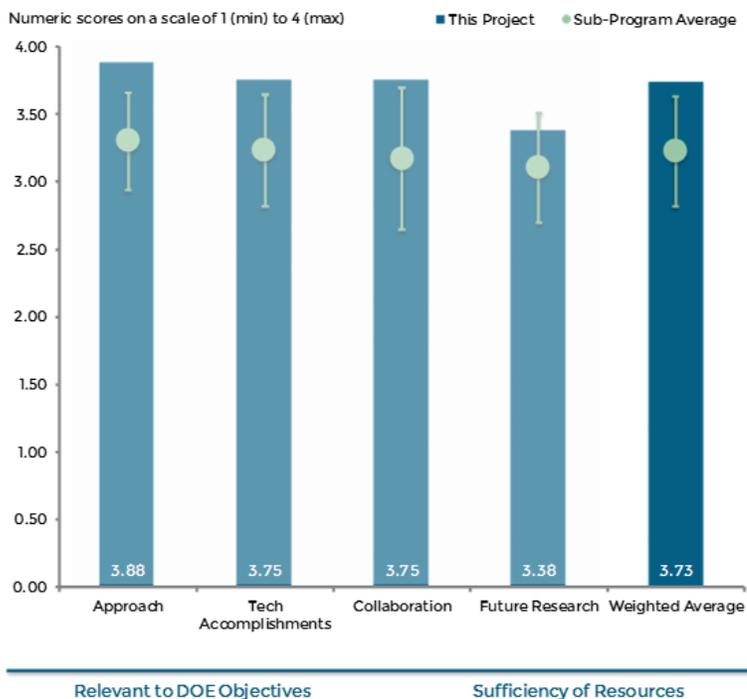
Reviewer 4:

The reviewer stated that the technical barriers are being adequately addressed, for these functional conductive polymers are of a new type and because of that new questions and potential new avenues of research can develop. The authors, however, are well focused on the program milestones.

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 towards DOE goals.

Reviewer 1:

The reviewer commented that the approach is very well focused and the experiments are systematically performed.



es223

Figure 2-41 Hierarchical Assembly of Inorganic/Organic Hybrid Si Negative Electrodes: Gao Liu (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer commented that the progress achieved so far is excellent and the developed binder is promising, but inquired if the binder can be applied to cathode to reduce mechanical stress caused life reduction related to cathode.

Reviewer 3:

The reviewer explained that the project team designed, synthesized the Polypyrrole (PPy) and demonstrated a good cycle life using the PPy conductive polymer binder and also using the hierarchical electrode design. However, the data will be more impactful if the loading was also presented along with the cycling data. The reviewer commented that the team should also report the rate used in their cycling tests with a good illustration of the pre-lithiation technique using the FMC stabilized lithium metal powder (SLMP).

Reviewer 4:

The reviewer observed that the project team has very interesting data obtained with the Polypyrrole PPy polymer, and that it is very surprising that the addition of a non-conductive functionality, in regards to DOE, does not hurt conductivity. The explanation based on a smoother film formation seems very appropriate, and the hierarchical electrode design seems to be a new concept. The reviewer added that using stabilized Li metal powder seems to be an interesting idea too.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that the project team has good collaboration with national laboratories and companies, and in addition, the role of each collaborator was clearly described.

Reviewer 2:

The reviewer commented that the authors have shown a strong collaboration with many institutions and clearly detailed their contributions.

Reviewer 3:

The reviewer stated that project team has good interaction with other team members and industries.

Reviewer 4:

The noted reviewer that there was a good collaboration for this project.

Question 4: Has the project 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 project team's future plans are good, but some of the cost involved with these polymers and the temperature effects should be addressed.

Reviewer 2:

The reviewer stated that as mentioned by the authors, the impact of additional conductive moieties should be pursued for it could be of interest to also investigate non-conductive moieties. At some point, the scalability of the process should be considered. The reviewer added that some information about the NMC powder that the authors are using is also important.

Reviewer 3:

The reviewer expressed that it is important to understand and further quantify the conductive polymer, but it is more important for the team to demonstrate as was proposed, a good cycle life using the proposed conductive

polymer binder but at a practical loading level of greater than 3 mAh/cm². In addition, the team should characterize the performance of the binder versus temperatures and rate in order to have more impact.

Reviewer 4:

The reviewer expressed that it is unclear how the binder performs in a wide temperature range and it is suggested to test the cell with the developed binder in a wide temperature range.

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

Reviewer 1:

The reviewer remarked that yes, the work is very much aligned with the objective of petroleum displacement, for a Si containing anode is very important for high-capacity batteries.

Reviewer 2:

The reviewer noted that this technology will help reducing the use of petroleum.

Reviewer 3:

The reviewer said that the successful development of a conductive binder will help to increase of battery life with Si electrode.

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 authors have been careful in staying on course, but may need additional resources if the team can expand their study into new areas that may develop during their research such as scale-up operations.

Simulations and X-ray Spectroscopy of Li-S Chemistry:
Nitash Balsara (Lawrence Berkeley National Laboratory) - es224

Presenter

Nitash Balsara, Lawrence Berkeley National Laboratory.

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:

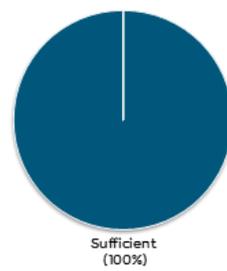
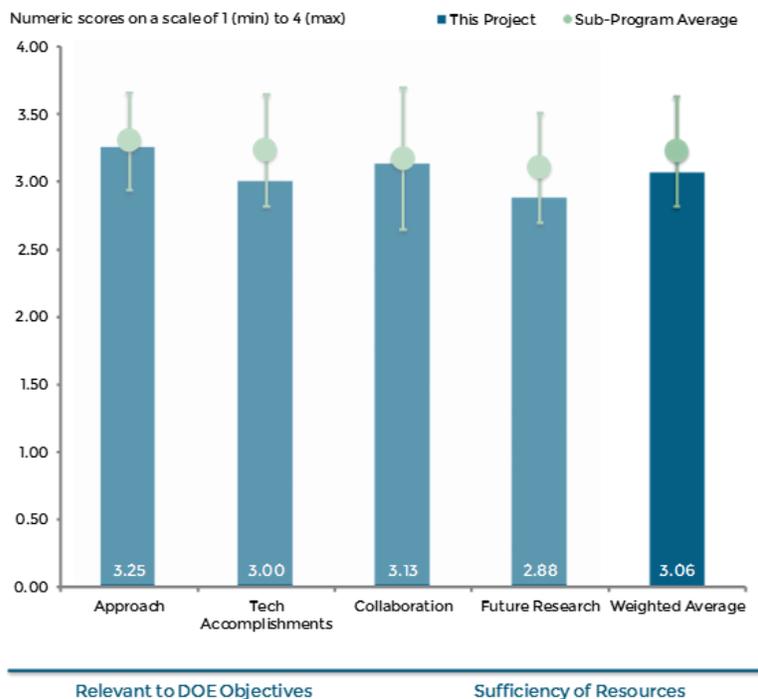
The reviewer pointed out that the first-principle simulation method has been used to aid the experimental characterization of reaction products, which helps provide new insight into the redox reaction pathways on the cathode side of Li-sulfur (S) batteries. The X-ray absorption spectroscopy (XAS) is the major characterization tool used in the project due to its unique characteristics. The reviewer suggested that the researchers comprehensively utilize other ex-situ or conventional microscopic and spectroscopic tools such as Raman, XPS, SIMS, SEM, HRTEM, STEM and EELS to provide the supporting evidence for identifying the intermediate and the final reaction products after operation of the cathode.

Reviewer 2:

The reviewer explained that the fundamentals of Li-S chemistry are well known for a long time, but the current project is trying to address the stability of the sulfides at various potentials that are important for Li-S battery. It is good to show that the stability of the sulfide species, but the project team should correlate with the sulfur dissolution.

Reviewer 3:

The reviewer stated that only the design of lithium sulfur cells with polyethylene oxide (PEO) cannot help in revealing the nature of the products produced during the electrochemical processes. Extending this interesting study to other type of electrolytes is recommended.



es224

Figure 2-42 Simulations and X-ray Spectroscopy of Li-S Chemistry: Nitash Balsara (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer explained that the results have demonstrated that the XAS and simulation can be successfully used for characterizing the intermediate and the final reaction products, and that the research could eventually unveil the redox reaction pathways on the cathode of Li-S battery. Identification of reaction products at the early discharge stage have shown some very interesting results. The reviewer expects that the redox reaction pathways on the cathode will be studied after or during the charge-discharge cycle, and it is interesting to check the products after different cycles of operation.

Reviewer 2:

The reviewer explained that the fact that the Li-S battery operated at 90°C can be misleading with regard to the produced products, although one can understand that with PEO there was a need for a high-temperature charging and discharging. In this case, it is recommended to look at a conventional electrolyte that can be used effectively at room temperature and perform the same XAS experiment for the purpose of comparison. The reviewer also stated that the team should be careful toward generalizing that the radical is generated during the early stage of the discharging process. This statement can only be true if the study were to be extended to other electrolytes.

Reviewer 3:

The reviewer commented that it would be helpful if the team can determine the precision and accuracy, as well as the detection limits, of polysulfides that can be measured by XAS combined with simulation. For example, the standard deviations should have been provided in the Table on Slide 13 of the presentation. The reviewer added that it would be valuable if the team can elucidate whether thermodynamics or kinetics is responsible for the absence of the reactions shown on Slide 15.

Reviewer 4:

The reviewer stated that it will be good if the PI can address the sulfur dissolution problem related to the stability so that the major issue of sulfur cathode dissolution can be explained, and that more experiments will be good in comparison to computation.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that the project has good teamwork.

Reviewer 2:

The reviewer said that the PI has addressed the previous review comments, and collaborated with other leading units to extend the research scope.

Reviewer 3:

The reviewer commented that project team needs more collaboration with the sulfur cathode group so that the PI can attack the specific issue in sulfur dissolution.

Reviewer 4:

The reviewer wondered if it is possible that too many collaborations would defocus the project, especially because many collaborators are outside of VTO.

Question 4: Has the project 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 it is very significant to conduct the XAS measurement of a cathode under the in-situ or operando condition. The effects of the charge-discharge process, the operating temperature, and the cycling on the reaction pathway can be clarified more clearly under the in-situ condition.

Reviewer 2:

The reviewer expressed that the project team use fundamental knowledge to build a Li-S cell with long cycle life and high-energy density, for enough experimental evidence is already present. The PI should discuss and collaborate with other lead researchers in the S area and try to help the issues such as sulfur dissolution.

Reviewer 3:

The reviewer said that more experimental work is needed, and that it is recommended to include low-temperature electrolytes to this work.

Reviewer 4:

The reviewer stated that the team should be more aggressive in using XAS to solve the polysulfide dissolution problem instead of just characterizing the problem.

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

Reviewer 1:

The reviewer stated that the ongoing research is well aligned with the mission and the objective of DOE program.

Reviewer 2:

The reviewer said that this project deals with the understanding of the Li-S battery, which the most important step before these kind of batteries can be suited for practical use.

Reviewer 3:

The reviewer noted that this work reduces the consumption of petroleum use.

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 reasonable resources are allocated to the project at this stage.

Design and Synthesis of Advanced High-Energy Cathode Materials: Guoying Chen (Lawrence Berkeley National Laboratory) - es225

Presenter

Guoying Chen, Lawrence Berkeley National Laboratory.

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 key focus areas of the work, such as understanding of phase transition, cathode and electrolyte interface, and transport limitations, received superb attention.

Reviewer 2:

The reviewer noted that that the project team has a good approach to synthesize single crystals and to understand the bulk versus surface effects on performance of the LMR-NMC high-voltage cathode.

Reviewer 3:

The reviewer said that the project team’s approach is solid and strong, but to meet DOE vehicle goals, electrode materials with high-energy density and high stability are required. Advances in materials development, therefore, require a better understanding of the relationships between electrode material properties and functions. The reviewer pointed out that the PI is removing the complexity of many similar investigations in the past by synthesizing well defined crystal systems. The advanced diagnostics, both ex-situ and in-situ, and experiments to characterize crystal properties and interfacial chemistry compliment the effort and will aid in the development of rationally designed 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 towards DOE goals.

Reviewer 1:

The reviewer described that the team has carried out high-quality studies to unravel the issues that plague the LMR-NMC cathodes, and that work on single crystals, especially the characterization studies using STEM and

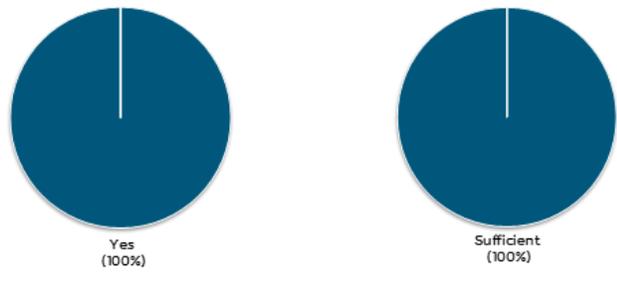
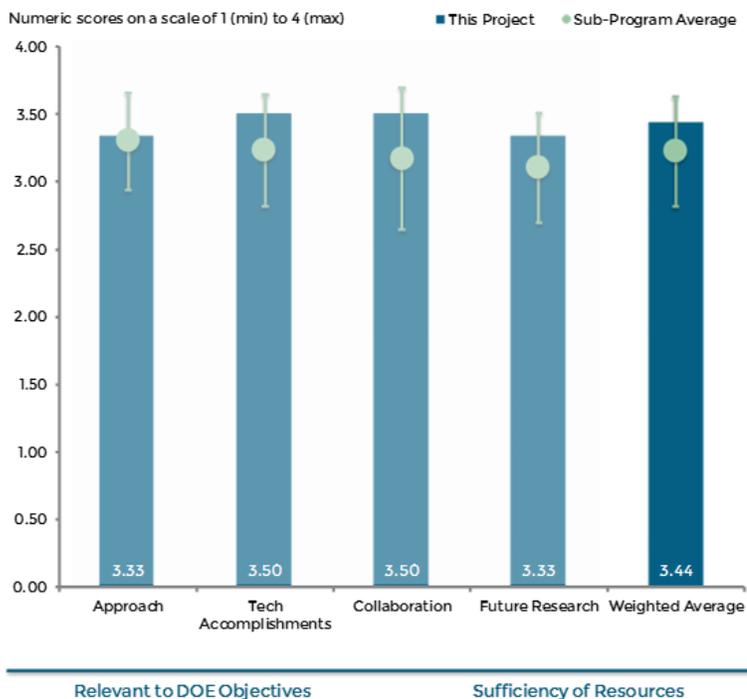


Figure 2-43 Design and Synthesis of Advanced High-Energy Cathode Materials: Guoying Chen (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

x-ray techniques, have been superbly carried out, and the results are really insightful. Transition metal (TM) dissolution and migration surface property characterizations have also been carried out superbly, and therefore, the resources are well spent.

Reviewer 2:

The reviewer stated that excellent progress was achieved this year, and that a host of LMR-NMC crystal samples were synthesized. The team revealed the contribution of key surface properties to the material challenges confronting the LMR-NMC cathode. In addition, diagnostic techniques were developed that can be used for single-particle based investigations. As a result of these efforts, there were numerous papers and presentations.

Reviewer 3:

The reviewer explained that a lot of data was presented on correlating surface morphology with performance, but it was not clear if the data was based on single cell or multiple cells per given type of surface morphology. The project team needed to provide statistics on the performance data in order to rank S-poly, L-poly and plate results and to identify one morphology with overall good performance. The reviewer said that some explanations are needed on how the surface spinel group affected the voltage fade which was thought to be induced by bulk structural change. The impact of electrode fabrication, for example, grinding, mixing, etc., on the morphology of the crystals, should be quantified since the morphology might not be maintained after the electrode fabrication and after the first activation charge when O₂ gas was evolved at high cut-off voltage.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that there is outstanding collaboration in this effort. The team consists of well-known scientists from Cambridge, University of California at Berkeley, University of California at San Diego, Oak Ridge National Laboratory (ORNL) and Pacific Northwest National Laboratory (PNNL).

Reviewer 2:

The reviewer stated that the project team has extensive collaboration with pertinent laboratories.

Reviewer 3:

The reviewer noted that the project team has good collaboration with national laboratories and companies.

Question 4: Has the project 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 list of future work is very extensive and hopes the authors continue to deliver the same high quality results as they have done during this review period.

Reviewer 2:

The reviewer remarked that these efforts will continue to further investigate the effect of synthesis and particle morphology on battery performance. The team will use the information to explore particle engineering to improve cathode performance and stability.

Reviewer 3:

The reviewer explained that proposed future work appeared to be a continuation of the fundamental characterization reported in 2015, but the proposed techniques to mitigate the cathode stability issue were vague. The project team needed to propose more specific surface modification techniques to improve the cathode stability by leveraging insights gained on the surface defect spinel.

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

Reviewer 1:

The reviewer remarked that definitely yes, the high-capacity cathode is the key to the development of high-energy batteries.

Reviewer 2:

The reviewer noted that the goals of this project are consistent with DOE Vehicle Technology 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 stated that that the funding level seems appropriate.

Microscopy Investigation on the Fading Mechanism of Electrode Materials: Chongmin Wang (Pacific Northwest National Laboratory) - es226

Presenter

Chongmin Wang, Pacific Northwest National Laboratory.

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 this project is developing a suite of advanced characterization and diagnostic tools to decipher how and why materials work. The in-situ and in-Operando tools developed by the PIs are especially important to the field, for the materials and issues they selected are all of high-importance to the DOE BMR programs.

Reviewer 2:

The reviewer commented that the approach has good combination of multiple diagnostics approaches to understand battery operation and degradation modes, and created three in-situ TEM tools.

Reviewer 3:

The reviewer stated that the PI used Operando HRTEM to probe the fading mechanism of Si anodes and high-capacity cathodes.

Reviewer 4:

The reviewer reported that the ex-situ, in-situ, and Operando HRTEM has been used to investigate the fading mechanism of electrode materials, and that so far, few studies have been performed on the electrode materials under the operando condition. The Operando HRTEM provides a unique approach for unveiling the time-resolved structure evolution on the nano-scale and atomic scale. The reviewer explained that this work is a big step forward in characterization of battery electrode materials, and that it is worth noting that the electrode materials are subject to bombardment of a high-energy electron beam during HRTEM observation. The reviewer was curious whether any damage of electrode materials was observed by the high-energy electron beam, and how such possible damage of electrode materials can be minimized or avoided completely.

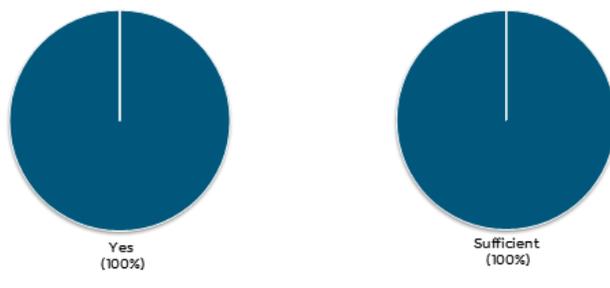
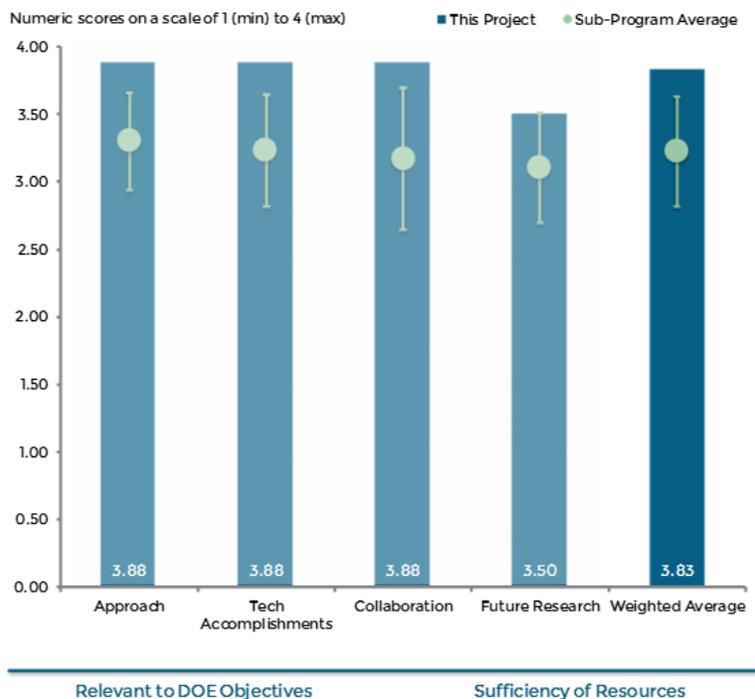


Figure 2-44 Microscopy Investigation on the Fading Mechanism of Electrode Materials: Chongmin Wang (Pacific Northwest National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer commented that the results obtained from the in-situ and Operando HRETEM experiments are very exciting, as for example, the HRTEM observation has found the gradual phase transformation C2/m to I41 to spinel in the $\text{Li}_{1.2}\text{Ni}_{0.2}\text{Mn}_{0.6}\text{O}_2$ electrode. The decrease in the Ni concentration inside the particle following cycling and the spatial partition of Ni and Mn at the edge indicate dissolution of Ni into electrolyte. The reviewer pointed out that the project team has also observed the oxygen loss and the Li depletion near the surface region in the Li_2MnO_3 electrode. These results have provided the direct evidence of electrode degradation, which will have important implication in designing electrode materials.

Reviewer 2:

The reviewer observed that the project team did a very nice demonstration that the O-layer on Si creates lithium oxide (Li_2O) when Si is lithiated, and though this has been understood for some time, it is nice to be shown. The project team has also investigated the function of an Alucone coated Si and shown how it impacts cycle life, but however, if Alucone consumes the silica oxide (SiO_x) particles, then one is probably losing active Li. The reviewer said that it would be interesting to investigate how to eliminate the silica oxide (SiO) from the anode material, to show surface segregation of Ni on LiNiMnO cathodes which is something that has been found in the past by Manthiram at Texas, and to also find dissolution of Ni into the electrolyte, similar to what was discovered on nickel cobalt aluminum (NCA) cathodes in the 2000 decade.

Reviewer 3:

The reviewer remarked that the PI's work on Si anodes and other cathodes is excellent, which included five papers published in high impact journals. The reviewer suggested that the team use closed cell to study surface sealed research, for the open cell is only suitable for internal structure study of the electrode, while the closed cell is suitable for the electrode and electrolyte interface study such as SEI.

Reviewer 4:

The reviewer stated that the PIs have completed the proposed milestone of devising liquid cells, which is of primary importance to the field. The SEI study on Si and Li protection and dendrite growth study under TEM would provide the most important info to the researchers in the area of BLI chemistries.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer commented that the PIs have demonstrated excellent collaboration with other laboratories, especially the material developers.

Reviewer 2:

The reviewer stated that the project team has very good collaboration with universities, national laboratories, and companies, but would like to see increased focus on problem solution, following the excellent problem elucidation demonstrated here.

Reviewer 3:

The reviewer said that the PI has collaborated with multiple national laboratories, universities, and instrument vendors, and that the collaboration is productive.

Reviewer 4:

The reviewer noted that the PI closely worked with other PIs in the program.

Question 4: Has the project 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 planned direction fits well with DOE's BMR focus and vision.

Reviewer 2:

The reviewer mentioned that to study SEI and coating on Si and LMR, NCM and NCA should use closed cell because it is related to the reaction to electrolyte.

Reviewer 3:

The reviewer explained that the proposed future work is timely and critical to the development of electrode materials, but the Operando cell under HRTEM needs a microfabrication facility. The reviewer asked if the PI has confirmed the availability of a microfabrication facility and necessary expertise. When a liquid cell is used under the HRTEM, the spatial resolution is reduced compared to the dry solid-state condition. The reviewer is curious about the best spatial resolution that can be achieved with the use of liquid cell.

Reviewer 4:

The reviewer was unsure that more work on Li dendrites is needed because there are already 30 years of work on that system, including diagnostics work. The reviewer liked the focus on understanding and trying to develop mitigation strategies for specific issues known to cause rapid capacity or power fade in high-energy electrodes.

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

Reviewer 1:

The reviewer noted that the ongoing research is well aligned with the mission and the objective of DOE program.

Reviewer 2:

The reviewer mentioned that the in-situ TEM study is important for understanding the mechanism of capacity decay due to the structure change of the electrodes.

Reviewer 3:

The reviewer remarked that yes, the work obviously supports 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 stated that the project costs are a very good value for a national laboratory, which is usually more expensive than \$200,000-\$300,000 per year.

Reviewer 2:

The reviewer said that the project's resources are sufficient.

Reviewer 3:

The reviewer noted that PNNL has the facilities for proposed research.

Reviewer 4:

The reviewer stated that no comments were necessary.

**BatPaC Model Development:
Shabbir Ahmed (Argonne
National Laboratory) - es228**

Presenter

Shabbir Ahmed, Argonne National Laboratory.

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 this is a well-focused project to develop design and simulation capabilities for assessing performance and cost of Li-ion batteries.

Reviewer 2:

The reviewer noted that there were vast model improvements in manufacturing assumptions and process improvements, which appear very logical and accurate. The depth of knowledge to support this model is apparent when reading of the process for recovery of volatile organic compounds (VOCs) or N-Methylpyrrolidone (NMP).

Reviewer 3:

The reviewer noted that the PI has the knowledge of the critical input needed for high reliability estimates for building a factory and processing operations to fabricate cell components.

Reviewer 4:

The reviewer reported that the approach taken to develop the Li-Ion BatPaC model contributes greatly to the improvement in performance and cost prediction of known battery chemistries, and it was clear that a lot of work went into the development effort for modeling both cell and to some degree battery pack costs. The approach to highlight manufacturing cost reduction methods and selecting a key process to address in presentation was great.

The reviewer expressed as one point for future consideration, there should be a clear indication of whether the data being presented is for a plant that builds battery cells, or a plant that builds battery packs and modules from cells. Slide 8 discusses a flex plant producing batteries, but the second bullet indicates that this plant actually produces cells. The next slide then discusses this same flex plant producing battery packs, and the following slide then indicates this is a cell plant as it talks about N-Methyl-2-pyrrolidone (NMP) recovery, which was a bit confusing. There were other instances of the information being great, but confusing in

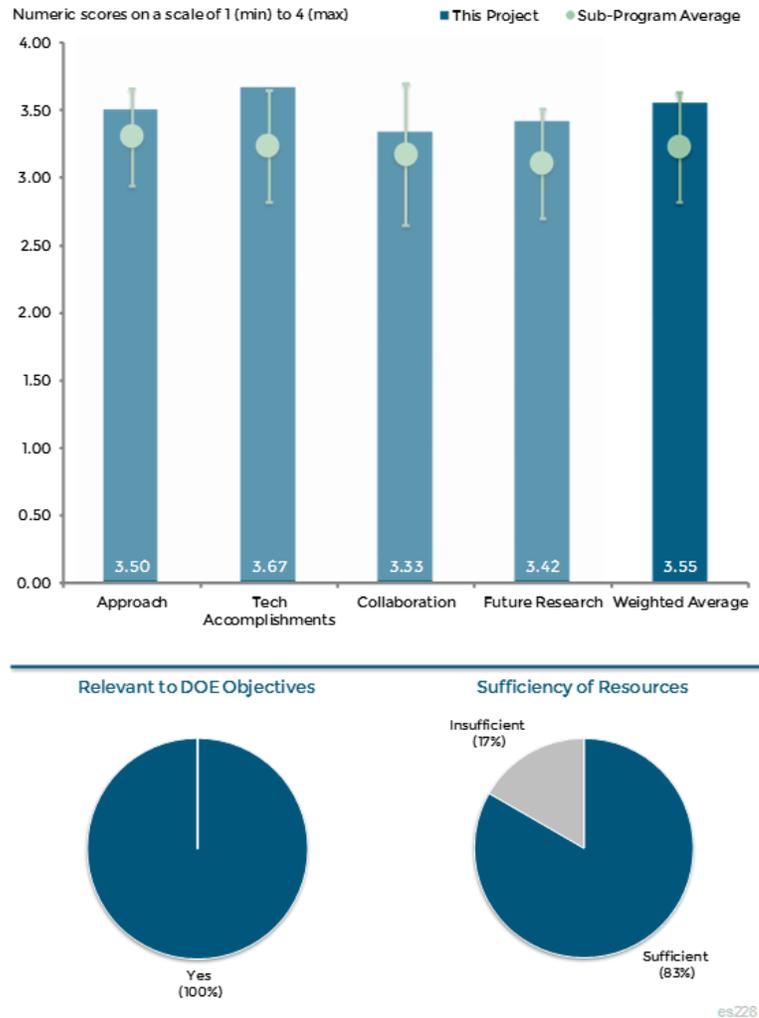


Figure 2-45 BatPaC Model Development: Shabbir Ahmed (Argonne National Laboratory) - Electrochemical Energy Storage

presentation. The reviewer thought Slide 13, for example, is great information for cell production. The reviewer unsure, however, of the value for a battery pack production facility.

The reviewer's assumption is that the information is for a cell manufacturer that produces the equivalent number of cells for this battery packs discussed, however this is not clear. The reviewer thought that the cell and battery terms are used interchangeably at times and that is where some confusion arises.

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 towards DOE goals.

Reviewer 1:

The reviewer reported that the presented data showed excellent progress towards the stated goals for this phase of program, which was good information for battery suppliers and users for identifying process change opportunities that could decrease overall cell production cost. The reviewer assumed that this information is for the battery cell manufacturers and those that track their cost, for cost savings to the cell manufacturer should ultimately result in cost savings to battery manufactures and users. This BatPaC model is of great value to automotive manufacturers of vehicles with electrified powertrains. The reviewer especially liked the analysis data that showed that a uniform electrode size (length and width) could be used for the cell for most batteries by just varying other cell characteristics, and how that would be a big cost savings.

Reviewer 2:

The reviewer stated that the flex-plant parameters will improve the factory cost estimates. The decision on using uniform electrode size of length and width, helps with the thickness of the electrodes.

Reviewer 3:

The reviewer noted that as being a BatPaC user, the progress is a good combination of user friendly and industrially relevant.

Reviewer 4:

The reviewer commented that the data obtained for the use of flex-line are very interesting if the footprints are closely matching, but is not sure how the changeover time was taken into consideration while calculating the cost or line efficiency. Line change could involve weeks of downtime. The reviewer added that the energy calculations for solvent recovery, and especially for dry-room operation, are very instructive and useful, and would like to know how many vendor responses were used to come up with these values.

Reviewer 5:

The reviewer stated that at the risk of redundancy to the prior question, this BatPaC model addresses the core processes and material assumptions that define the Li-ion battery (LIB), and therefore, barriers can be identified and addressed. As LIB technology is core to DOE energy storage goals, this type of project is clearly at the core of DOE's goals.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that project team's collaboration has been excellent.

Reviewer 2:

The reviewer pointed out that the project has utilized key and industry leading collaborators such as LG Chem, General Motors Company, 3M Company, and others to define assumptions, processes, and validate assumptions, and could not think of a better collaboration.

Reviewer 3:

The reviewer described that project team's collaboration with significant high-volume cell manufacturers, via confidential information exchange agreements to include more real-world information, could be an improvement opportunity towards greater level of output reality. This work may be best accomplished by organizations outside of ANL, which can give best assurance to collaborators of information protection, while still allowing ANL modelers to the access of their generalized model data.

Reviewer 4:

The reviewer stated that collaboration partners included cell materials developers and manufacturers as well as battery manufacturers, and also one of the world's largest automotive battery users. This type of collaboration is needed to keep this effort up to date and moving forward.

Reviewer 5:

The reviewer commented that the partners are the battery developers and producers who will be able to validate the model.

Reviewer 6:

The reviewer noted that high-volume battery producers were conspicuously absent.

Question 4: Has the project 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 continuing research will make the model more useful.

Reviewer 2:

The reviewer explained that as was stated prior, and to have worked with the model years ago, one can witness increased fidelity to the processes and associated barriers. Through this timed perspective, one can see the great thought that has entered the logic flow for model maturity.

Reviewer 3:

The reviewer commented that because all suppliers are moving towards single cathode systems, it will make sense to carry out the studies with blended cathode systems, and recommended expanding the future collaboration to include low-cost suppliers in China who increasingly play a big role in component sourcing. The reviewer asked if energy calculations will also be done for formation systems.

Reviewer 4:

The reviewer stated that the cathode work is heavily weighted in this model as compared to the other cell components, and that the other cell components need more attention, the anode and separator in particular. There was no clear indication of the effort that would be expended toward the analysis of these other components in future work, and no clear mention on directional information for cell format and tab designs being added to the model. The reviewer commented that this would also be very helpful for both cell manufacturers, battery pack builders, and automotive customers.

Reviewer 5:

The reviewer would like to hear more on other cell formats and capacity.

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

Reviewer 1:

The reviewer remarked that yes, the work does support DOE objectives. Having a reliable cost model especially those that deal with the use-line efficiency and energy consumptions, are very useful for developing cost-effective cells and batteries.

Reviewer 2:

The reviewer explained that the BatPaC model helps identify ways that a cell manufacturer can realize a meaningful cell cost reduction, for the cell cost is at least 50% of an automotive battery cost. Cost is one of the biggest hurdles for adoption of this technology as a viable alternative to the ICE, and consequently, any system that allows for a meaningful cell-cost reduction supports the DOE objective to reduce petroleum usage.

Reviewer 3:

The reviewer reported that this BatPaC model addresses the core processes and material assumptions that define the LIB, and therefore, barriers can be identified and addressed. As LIB technology is core to DOE energy storage goals including petroleum displacement, this type of project is clearly at the core of DOE goals.

Reviewer 4:

The reviewer noted that the optimized cost and performance estimate help the cell developers produce and sell batteries to the automotive OEMs.

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 this project seems to have a good return on investment (ROI) and warrants future updates and support.

Reviewer 2:

The reviewer stated that the resource support of the ANL modelers and the industry will be sufficient to achieve the milestones.

Reviewer 3:

The reviewer stated that the resources provided to the project should be sufficient to meet the stated milestones.

Reviewer 4:

The reviewer commented that project's funding level seems to be okay.

Reviewer 5:

The reviewer noted that any signs of project funding short-falls or excesses are not apparent.

Lithium-Ion Battery Production and Recycling Materials Issues: Linda Gaines (Argonne National Laboratory) - es229

Presenter

Linda Gaines, Argonne National Laboratory.

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 said that the project is well-planned, comprehensive and has very focused goals.

Reviewer 2:

The reviewer stated that the project objectives are clearly identified as well as having potential methods to address them, as production and recycling of Li-ion batteries are two very big issues that are being addressed. The approach to address these issues and their impact on the environment was very inclusive and made use of the tools and information available. The reviewer, however, would have liked to have seen more involvement from battery users.

Reviewer 3:

The reviewer noted that the battery manufacturing issues similar to energy consumption are being addressed along with the difficulties in recycling.

Reviewer 4:

The reviewer stated that this subject matter is difficult and complicated, but essential for success of the LIB technology. This work has been an arduous and lengthy process since 2008. Therefore, in the bigger picture, the reviewer wants to understand how this work is going to close the loop and be used to drive decisions in LIB development in both industry and future DOE program definitions.

Reviewer 5:

The reviewer commented that the approach is otherwise excellent except for three issues; First, the reviewer noted many references and comparisons to lithium cobalt oxide (LCO) cathode material. The reviewer asked if it is used in automotive applications at all. If not, then if a comparison is made, it should be noted that it is used in consumer electronics applications included only as a reference due to high-volume usage in non-automotive

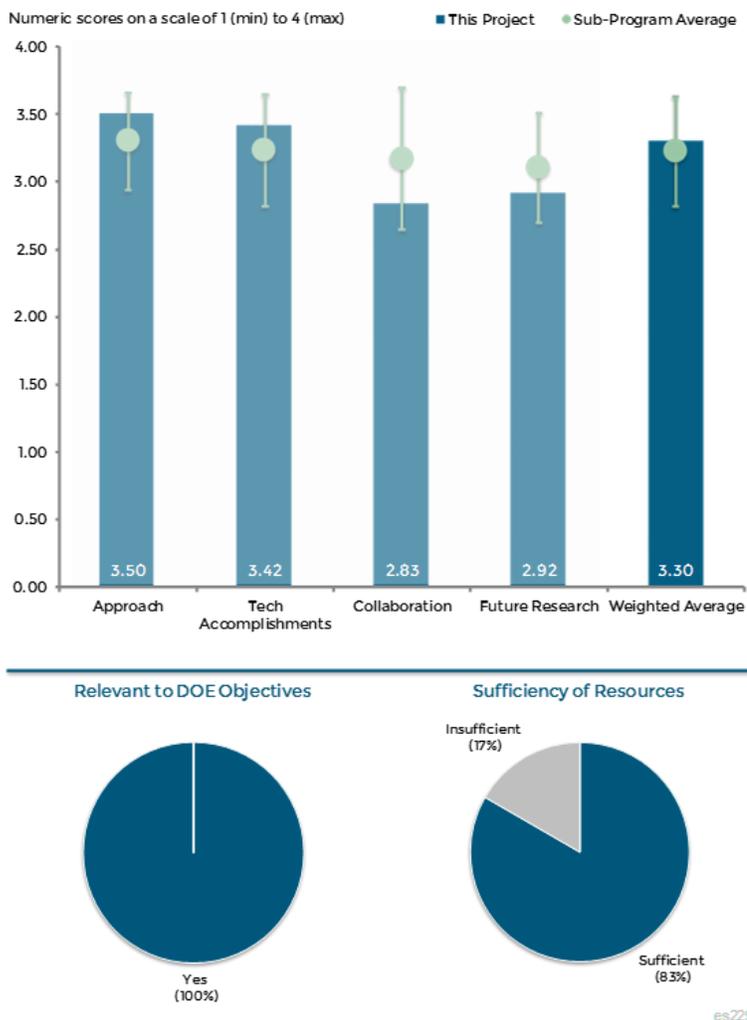


Figure 2-46 Lithium-Ion Battery Production and Recycling Materials Issues: Linda Gaines (Argonne National Laboratory) - Electrochemical Energy Storage

applications. The reviewer remarked that the second issue is that the intermingling of Li-ion into lead-acid battery recycling is important issue, but asked if this work is doing anything to contribute to resolution of this issue from a scientific or technical perspective. If nothing, then it seems like using project is to promote industry special interests and hype. Thirdly, the reviewer commented that a portion of activity in this particular project involving the study of cathode exposure to acids or bases seems inappropriately primitive. Argonne should be capable of something much more relevant and insightful.

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 towards DOE goals.

Reviewer 1:

The reviewer noted that the team has been generating a lot important and relevant data from material availability, recycling, and energy consumption points of view. These are very useful and much appreciated, and the PI's work is a great source of valuable information.

Reviewer 2:

The reviewer reported that project team's nearly outstanding progress is an excellent accomplishment. The reviewer had one comment on Slide 13. It was not very clear whether this was related to the mining of the material, the recovering of the materials from a recycled product, or from both. There is a good summary on battery life-cycle impact on environment, and the project shows areas of opportunities for improvement for both carbon dioxide (CO₂) and sulfur oxides (SO_x) emissions reductions. The reviewer said it would be good for a separate study to identify potential ways to reduce even further the plant CO₂ emissions, and identify ways to reduce the SO_x emissions during carbon monoxide (CO) and Ni mining operations assuming that the mining operation is the biggest contributor to this SO_x emission. The reviewer added that the project team has a really good analysis showing various recycling methods and how they impact energy usage and emissions generation.

Reviewer 3:

The reviewer noted that the detailed cradle-to-gate analyses and comparisons are useful, and that the project team has excellent accomplishments given the budget of the program.

Reviewer 4:

The reviewer commented that contacts have been established to complete the task.

Reviewer 5:

The reviewer asked what usage metric is used to define the baseline for the analysis, or what volume and ramp rate by 2050, in terms of the material scarcity. The reviewer was pleased to see that the BatPaC and Greenhouse Gas, Regulated Emissions, and Energy Use in Transportation (GREET) models are publically being utilized for other than U.S. Environmental Protection Agency (EPA) or CAFE analysis.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that the project team has excellent collaboration given the size of the budget.

Reviewer 2:

The reviewer remarked that additionally, Toxco (Retrieve) might be added as a collaboration partner because the company is already helping the battery industry to recycle some of the chemistries.

Reviewer 3:

The reviewer explained that from the material scarcity and battery production perspective, this project may consider additional industry partnerships that have performed similar analysis with financial risk. The reviewer said that if from the recycling perspective, arguably the most important portion of this project, if the project

team has considered analysis beyond the technical and economic perspective, for example, from governmental policy on a world-wide basis.

Reviewer 4:

The reviewer expressed that encouragement for a much wider collaboration with material vendors and manufacturers, especially those in Japan and China, to obtain process info and cost for having improved reliability.

Reviewer 5:

The reviewer would like to see more involvement with automotive battery users, for the involvement of the EPA or other regulatory type organizations was not clearly stated, for their direct involvement would have been great, if possible.

Reviewer 6:

The reviewer noted that the project team did not cover much collaboration in the presentation.

Question 4: Has the project 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 program recognizes the ongoing work that is needed and the appropriate modeling tool needed support, where future work appears to include the effort to improve process development, but the key development areas were not clearly and sufficiently identified. Looking at using recycled batteries from consumer devices as feedstock for inclusion in the development of automotive batteries is good. The reviewer would like to see support from automotive OEMs and strong Li-ion battery suppliers included, and how environmental agencies support this effort in some way, as well as SAE or similar organizations. Finally, there should be some effort added to identify non-intrusive ways to strongly encourage the return and collection of the used consumer and other Li-ion battery cells and batteries.

Reviewer 2:

The reviewer stated that future research should include alternative demand of cathode materials for consumer battery using the automotive recycled batteries.

Reviewer 3:

The reviewer commented that perhaps redundant to a prior statement, there is a desire that a closing of the loop must be accomplished to complete this work.

Reviewer 4:

The reviewer is keen on learning how these future estimations are affected when one also considers batteries for energy storage use.

Reviewer 5:

The reviewer commented that there is not much detail on future work in the presentation.

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

Reviewer 1:

The reviewer said that this project work is a highly relevant topic because life-cycle assessment (LCA), recycling of batteries, and energy consumption of various processes are critically interrelated to the DOE objectives.

Reviewer 2:

The reviewer reported that this work strongly supports the DOE objective to displace petroleum usage, for the recycling cost of these batteries could become a defining barrier or become an environmental disaster because of cost to the end user. Customers may decide to not purchase battery powered vehicles because the recycling cost could be as much as 10% of the initial battery cost.

Reviewer 3:

The reviewer remarked that yes, the project supports the DOE objectives because it is working on the enablers of electric storage technology.

Reviewer 4:

The reviewer noted that the cost of recycling will help with the cost estimation of new batteries and justify for more effective use of the automotive EV 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 explained that there are many different directions for this project to be expanded that will reduce the overall cost for the industry at both the vehicle OEM and consumer usage levels. Additionally, more funding is needed to reduce the potential negative environmental impact today, in the near future, and in the relatively near term future. The reviewer added that these are the reasons that one thinks that more funding is needed in this area.

Reviewer 2:

The reviewer commented that the project team has pretty good judgment in managing scope and mission creep.

Reviewer 3:

The reviewer noted that the ANL researchers and the industry partners will help with the resource issues.

Sulfur Cathode for Lithium-Sulfur Batteries: Yi Cui (Stanford University) - es230

Presenter

Yi Cui, Stanford University.

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 reported that the approaches are well outlined in a comprehensive fashion, where experiments combined with simulation have been used to develop the cathode and microscopic characterization and electrochemical testing have been utilized to evaluate the cathode. The reviewer also commented that it would be good if the principle and rational for material design are elaborated and justified.

Reviewer 2:

The reviewer stated that the approach of making nano-sulfur and the architecture is good, but the PI should focus on attacking one architecture instead of several structures.

Reviewer 3:

The reviewer said that the approach is relevant although one can argue that the inclusion of an electrolyte study could make this study more comprehensive.

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 towards DOE goals.

Reviewer 1:

The reviewer pointed out that outstanding results have been obtained in a systematic way, and that the extension of the study to lithium sulfide was a good move. Sulfur cathode development is important, however, it is recommended to include some electrolyte related work.

Reviewer 2:

The reviewer explained that several composites including the hydrogen-reduced titanium dioxide (TiO_{2-x}) inverse opal sulfur, the Magnéli-phase TiO_{2n-1} nanomaterial, the hollow S-amphiphilic polymer nano-

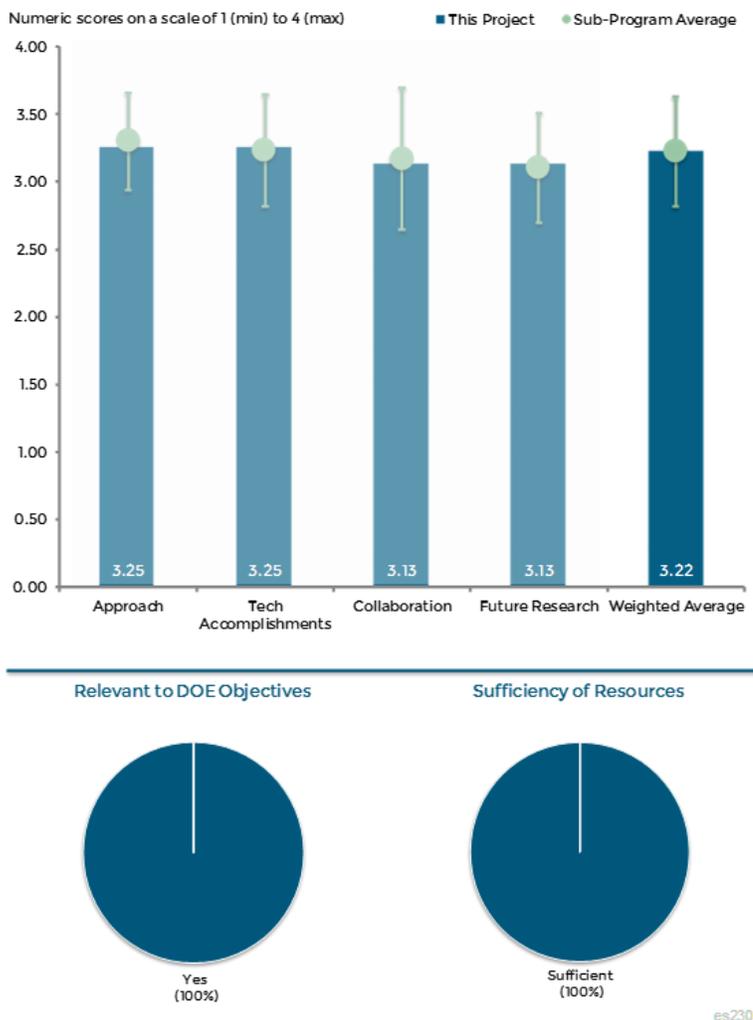


Figure 2-47 Sulfur Cathode for Lithium-Sulfur Batteries: Yi Cui (Stanford University) - Electrochemical Energy Storage

particles, and the conductive polymer-coated hollow sulfur have been developed, and that such scaffolds or coatings for the sulfur cathode have improved the cyclic stability significantly. The reviewer said that it would be great if the PI can address the common and the difference in the rationale for designing different composites. The focus of this project is on the development of cathode material, but the match between the cathode material and the electrolyte needs to be considered in order to optimize the performance of a full cell. The reviewer is eager to check how the PI addresses this point when developing composite cathodes.

Reviewer 3:

The reviewer stated that several nano materials have been proposed and studied, but all of them seem to have the same problem; S dissolution is the common problem. Though publication is important, it is better to focus on one system and understand it well, rather than publishing several papers.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the PI has recruited some collaborators with the expertise complementary to the PI, and has organized a productive, well-coordinated multidisciplinary research team.

Reviewer 2:

The reviewer commented that the PI has a good team.

Reviewer 3:

The reviewer remarked that the PI indicated no clear collaboration.

Question 4: Has the project 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 future plan has been well articulated, even though it still remains a challenge to develop a S cathode with a high density, and which is capable of excellent rate capability while maintaining good cyclic stability. To conduct research toward this direction is interesting.

Reviewer 2:

The reviewer said that the PI's future plan is sound.

Reviewer 3:

The reviewer commented that the volumetric efficiency should be a focus of the future work, and that the cycle life and failure mechanisms of balanced full cells, for example, without the unlimited supply of Li, should also be investigated and reported.

Reviewer 4:

The reviewer explained that the proposed future work describes the issues to be addressed, but the main challenge of preventing the active S species from diffusing into the electrolyte, is not addressed. This is critical for the future use of S cathode.

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

Reviewer 1:

The reviewer said that the ongoing research is well aligned with the mission and the objective of DOE program.

Reviewer 2:

The reviewer explained that although this S battery project is still basic in nature, the information learned may help solve the inherent issues known in Li-S sulfur batteries.

Reviewer 3:

The reviewer noted that this technology will help in reducing 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:

The reviewer stated that adequate resources have been allocated.

Reviewer 2:

The reviewer noted that the resources are sufficient.

Reviewer 3:

The reviewer remarked that no further comments are needed.

High Energy Density Lithium Battery: Stanley Whittingham (Binghamton University) - es231

Presenter

Stanley Whittingham, Binghamton University.

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 it is good to see some creative approaches to high-energy density, and refreshing that the choices were made as alternatives to Si anodes and nickel rich intercalation cathodes. The project is in its early days, but it has a good start to begin to understand some of the interesting alternatives.

Reviewer 2:

The reviewer remarked that the approach in this project is outstanding. The research conducted may potentially result in new anode and cathode to replace current carbon anode and cathodes.

Reviewer 3:

The reviewer pointed out that project team's approach has innovative concepts to potentially overcome traditional barriers, but much testing and evaluation is needed to show how barriers are to be overcome. The approach could include HQ nano-Si materials as an alternative anode technology, where HQ would provide the materials, and that clear goal to achieve 300 Wh/kg and low-cost.

Reviewer 4:

The reviewer stated that the critical problem for copper (II) fluoride (CuF_2) is the dissolution and migration of copper (Cu) which results in fast capacity decay. The PI should focus on this critical problem. This reviewer added that M-Sn-C alloys have been investigated for Li-ion battery anode, although the innovation of this study is not clear.

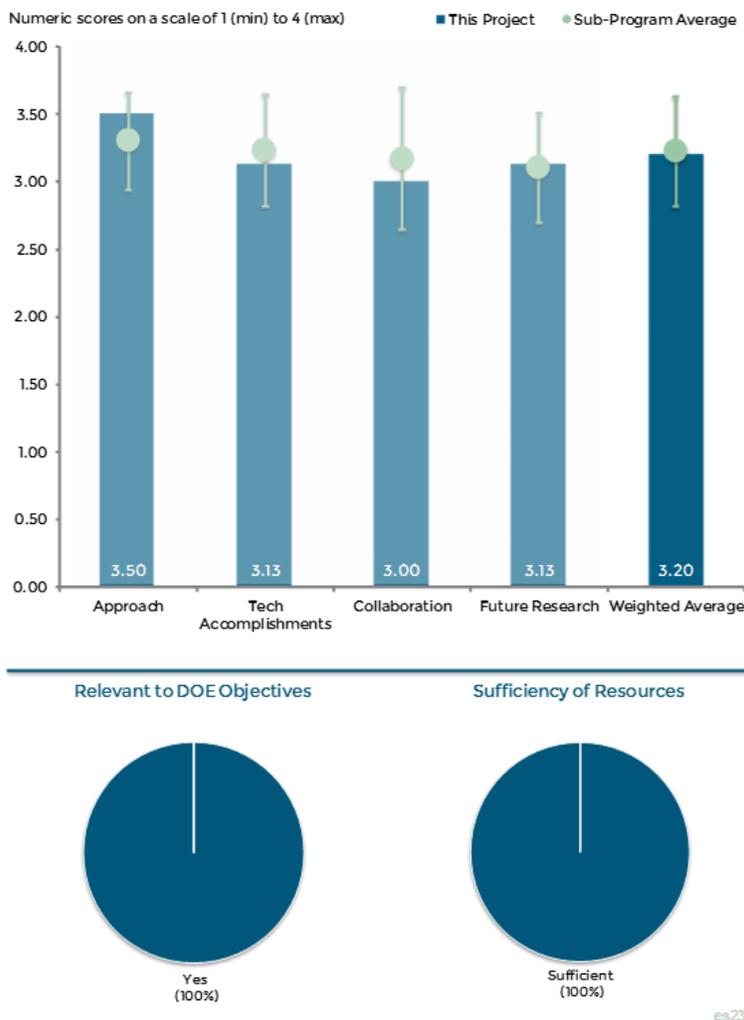


Figure 2-48 High Energy Density Lithium Battery: Stanley Whittingham (Binghamton University) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer said that the technical achievement is excellent for this project so far.

Reviewer 2:

The reviewer noted that project is in its early days, but the progress appears appropriate for the time period.

Reviewer 3:

The reviewer commented that progress has a long way to go in showing how classical barriers are overcome by these new materials. Overall strategy is robust in that both intercalation and conversion materials are considered.

Reviewer 4:

The reviewer described that the PI should focus on critical challenges of CuF_2 dissolution and aggregation, for Sn-iron (Fe)-C alloys, dissolution of SEI may contribute the capacity if the alloys are charged and discharged in the tin 0.0-3.0 V window, and added that because the PI did not provide the charge and discharge curve, it is hard to evaluate. The high-irreversible capacity is another issue for ball-milled Sn-Fe-C alloys.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the PI has appropriate technical collaborations to achieve the project objectives. Involvement with New York Battery and Energy Storage Technology Consortium (NYBEST) is unique and could result in more collaboration and funding.

Reviewer 2:

The reviewer noted that the PI is collaborating with the scientists in Brookhaven National Laboratory (BNL), ANL and NYBEST.

Reviewer 3:

The reviewer said that again, the project is in its early development. Collaboration will be more important as development moves into more complex materials development and into more complex cell configurations.

Question 4: Has the project 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 proposing the innovative materials is a good strategy, but it has to be backed up by extensive and convincing testing.

Reviewer 2:

The reviewer stated that it will be interesting if there is an impact of electrolyte at higher temperature to cyclability with the CuF_2 electrode, and if a failure modes study such as structure change of electrode materials, can be included in the future research plan.

Reviewer 3:

The reviewer noted that the capacity decay mechanism should be investigated for CuFe_2 .

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

Reviewer 1:

The reviewer stated that alternative high-capacity anodes and cathodes are important activities in high-capacity cell development.

Reviewer 2:

The reviewer said that the project has a good potential to improve battery performance and broaden

Reviewer 3:

The reviewer stated that this project addressed the target set by DOE on energy storage and tried to attack the technical barriers to increase battery energy density and reduce cost.

Reviewer 4:

The reviewer noted that the research fit the DOE 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 said that more resources will be necessary in a more mature state.

Reviewer 2:

The reviewer stated that the PI has the required capability to conduct proposed research.

Reviewer 3:

The reviewer stated that project's resources are currently adequate.

Electrode Fabrication and Performance Benchmarking: Vincent Battaglia (Lawrence Berkeley National Laboratory) - es232

Presenter

Vincent Battaglia, Lawrence Berkeley National Laboratory.

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 pointed out that the PI optimized the electrode components and processing to achieve high-energy density and cycle life.

Reviewer 2:

The reviewer commented that the approach of this project is to provide quality electrodes and determine the electrode failure mechanism.

Reviewer 3:

The reviewer stated that it is important to have an independent capability to build electrodes and cells as a third-party independent evaluation of material capability. There is much good work here but perhaps a little unfocused as to supporting a clear charter or mission.

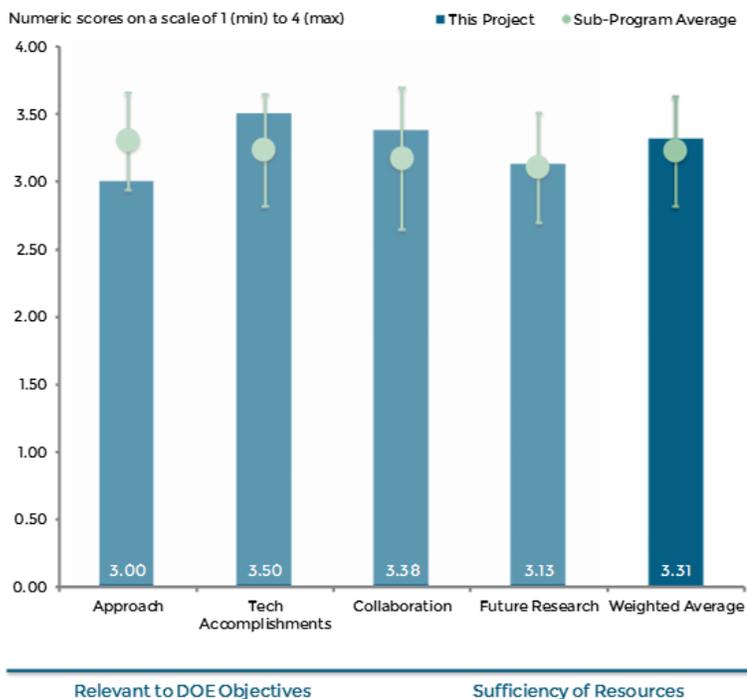
Reviewer 4:

The reviewer noted that approach demonstrated the test for various quality electrodes and their failure mechanism.

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 towards DOE goals.

Reviewer 1:

The reviewer remarked that again, the approach has some very interesting and wide-ranging data. The downside is that it perhaps lacks a bit of clarity on an overall objective.



es232

Figure 2-49 Electrode Fabrication and Performance Benchmarking: Vincent Battaglia (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer explained that the reference position outside the anode and cathode cause abnormal impedance for anodes. The PI should validate if the electrochemical impedance spectroscopy (EIS) sum of the anode and cathode should be equal to the EIS of the two-electrode full cell.

Reviewer 3:

The reviewer expressed the need to know if there are any other physical and chemical means that can be used to determine a failure mechanism in addition to impedance and charge and discharge testing.

Reviewer 4:

The reviewer expressed the need to understand why lithium iron phosphate (LFP) electrodes cannot be made for 0.8 mAh/cm² without cracks, and that failure mechanisms should be further examined.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team has a good collaboration and interaction.

Reviewer 2:

The reviewer noted that this work is collaborative.

Reviewer 3:

The reviewer said that the work relies on expanded collaboration within existing programs to evaluate materials early in the development program and to allow for benchmarking of the progress of advanced materials.

Question 4: Has the project 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 Slide 36 summarizes all the issues to be addressed, and that this project should be further continued in order to understand the failure mechanism.

Reviewer 2:

The reviewer expressed a need to know if there are any alternative solutions to the challenges and barriers identified in this project.

Reviewer 3:

The reviewer commented that not much work can be done during the three remaining months.

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

Reviewer 1:

The reviewer stated that optimization of the cell is also important for the full use of the electrode materials.

Reviewer 2:

The reviewer said that this project provided quality materials to support the BMR program.

Reviewer 3:

The reviewer noted the project work will reduce the use of petroleum.

Reviewer 4:

The reviewer expressed an agreement with the concept of an independent capability to build and evaluate cells with small materials amounts.

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

Reviewer 1:

The reviewer observed that the PI can do the proposed work at LBNL.

Efficient Rechargeable Li/O₂ Batteries Utilizing Stable Inorganic Molten Salt Electrolytes: Vincent Giordani (Liox) - es233

Presenter

Vincent Giordani, Liox.

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 reported that this project is addressing a key issue with Li-air systems, and that is the formation of non-reversible Li salts. The project team has developed a strong testing protocol to help with the characterization efforts, and has shown the ability to detect and characterize the key impurities and products. The reviewer commented that a bit more background on the topic would help in future presentations.

Reviewer 2:

The reviewer stated that the PIs explored the use of a molten salt electrolyte for Li-air batteries, and that the electrochemical stabilities and thermo-characteristics of the electrolytes were investigated. Li peroxide (Li₂O₂) and O₂ solubility and diffusion coefficients were also measured, and the Li-air performance was tested. The reviewer added that the approaches are solid and aim to understand the fundamental aspects of O₂ redox reaction in molten salt.

Reviewer 3:

The reviewer noted that the project team has an interesting approach to solving the rechargeability problem in the Li/O₂ system.

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 towards DOE goals.

Reviewer 1:

The reviewer reported that there was a significant drop in transference with the eutectic electrolytes and this could be a significant issue. At this point, the project to appears to have been running a large number of characterization tests, and while appropriate, it is unclear if the full battery work was necessary before material

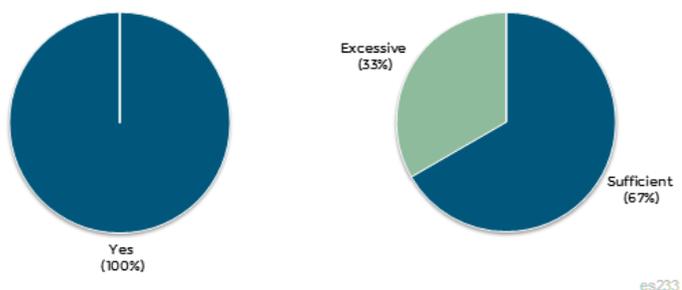
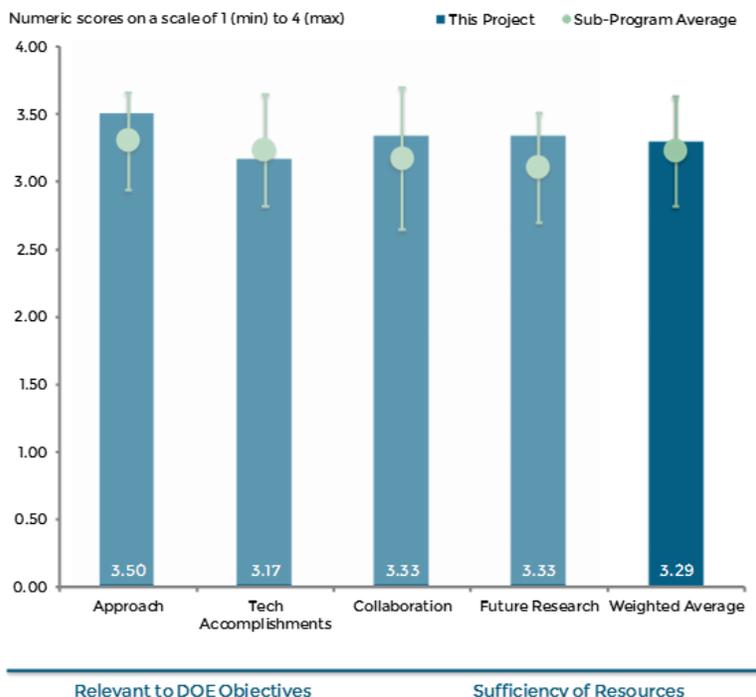


Figure 2-50 Efficient Rechargeable Li/O₂ Batteries Utilizing Stable Inorganic Molten Salt Electrolytes: Vincent Giordani (Liox) - Electrochemical Energy Storage

choices had been narrowed down. The reviewer observed that all project milestones have been hit to date though to this point, there has been little novel work. One can understand that most of the work to this point involved set-up, and it will be curious to see how future work develops. The reviewer went on to say that it was quite interesting to see how with precise O_2 measurement, the team was able to measure the number of electrons.

Reviewer 2:

The reviewer explained that the PIs accomplished the milestones on time and that the critical aspects of the systems were investigated. However, the electrochemical results, for example, the high round-trip efficiency, need to be confirmed with gas analysis in order to make sure that the oxidation reaction was indeed the oxidation of Li_2O_2 . The reviewer added in addition, because the solubility of O_2 and Li_2O_2 are so low in the molten salt, the PIs need to comment on the rate of the reaction (charge and discharge rate).

Reviewer 3:

The reviewer stated that more emphasis should be made on studying compatibility of all cell components with the molten salts, and that it would be interesting to see an assessment of the volumetric energy density on a system level for the proposed system versus the original electrolyte system.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the collaboration with LBNL and Caltech demonstrates a strong coordination of the research. It seems such collaboration could result in more results, for example, the proposed in-situ gas analysis.

Reviewer 2:

The reviewer noted that collaborators are best in this research area.

Reviewer 3:

The reviewer said that the collaborations with Lawrence Berkeley National Laboratory (LBNL) and Caltech are appropriate, and that given the early status of the technology, it would be important to have discussions with the wider Li-air community but something formal is not expected.

Question 4: Has the project 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 set-up of the testing sensor bodes are well used for the expedited development of a non-carbonaceous electrolyte for Li-air, though a more detailed plan on this would have been appreciated. The project team has good eye-to-technology commercialization, which should help ensure the impact after the research is completed. The reviewer added that there needs to be focus on the impact of this work on the full system metrics.

Reviewer 2:

The reviewer commented that it will be beneficial to add a task on studying the Li anode and the molten electrolyte system for the rechargeable Li systems.

Reviewer 3:

The reviewer said that the proposed future work for non-carbon electrode selection and management of Li_2O_2 dissolution and precipitation are in a solid direction. The reviewer suggested that the co-PI in LBNL should do more analytical investigation to understand the true nature of the redox reaction.

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

Reviewer 1:

The reviewer said that the project has a potential to benefit Li-based rechargeable systems.

Reviewer 2:

The reviewer stated that the development of higher energy density, lighter weight, and longer cycle life batteries would accelerate the electrification of the transportation sector.

Reviewer 3:

The reviewer noted that the research is very relevant to the DOE 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 noted that the PIs have adequate resources for the research.

Reviewer 2:

The reviewer pointed out that about one-third of the project's budget has already been spent while one-sixth of the project is complete. This observation merited a discussion and that an explanation would have been appreciated.

Continuum Modeling as a Guide to Developing New Battery Materials: Venkat Srinivasan (Lawrence Berkeley National Laboratory) - es234

Presenter

Venkat Srinivasan, Lawrence Berkeley National Laboratory.

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 PI has an excellent approach where relevant problems are attacked in a number of areas important to advanced battery development.

Reviewer 2:

The reviewer explained that the combination of x-ray tomography with three-dimensional (3D) microstructure simulations will lead to promising new insights. The reviewer expressed the need to know if microstructure change due to aging will be included in the future work.

Reviewer 3:

The reviewer noted that approach has a good marriage between modeling and experimental work.

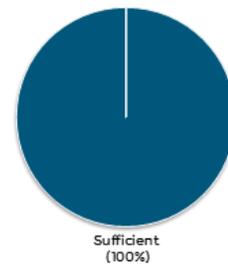
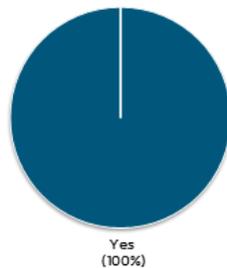
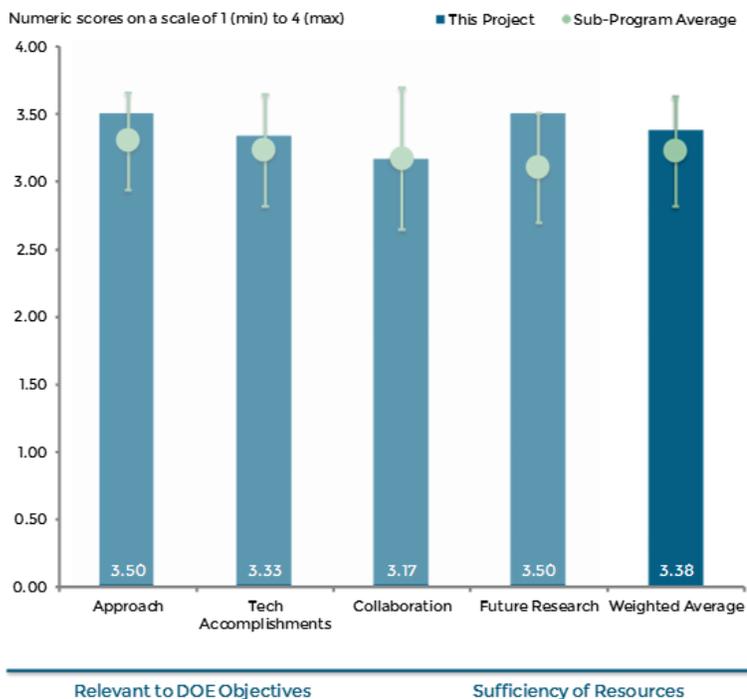
Question 2: Technical Accomplishments and Progress toward overall project and DOE goals—the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals.

Reviewer 1:

The reviewer remarked that project team has excellent progress towards improving the model through a careful and deep understanding of the input parameters.

Reviewer 2:

The reviewer stated that the simulation work at cell level for the Li-S battery is inspiring. More discussions on the over-all energy density at the cell level, not just energy density normalized by active materials, can help the decision making for vehicle development.



es234

Figure 2-51 Continuum Modeling as a Guide to Developing New Battery Materials: Venkat Srinivasan (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

Reviewer 3:

The reviewer expressed that a number of the PI's results were quite interesting, especially favoring the PI's conclusions about Li conducting glasses.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the PI has several collaborations, but almost all of them are within his laboratory.

Reviewer 2:

The reviewer commented that good collaboration is that best blend of theoreticians and practitioners.

Question 4: Has the project 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 PI plans to continue the project's present development and to extend its studies into new areas.

Reviewer 2:

The reviewer said that future work includes broad selections of systems and tools.

Reviewer 3:

The reviewer expressed to know what the follow up work is for Si and binder simulation.

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

Reviewer 1:

The reviewer commented that this project could lead to a broad range of advanced battery improvements. Ultimately, this will lead to reduced battery costs enabling further electrification of the nation's vehicles and improved gas mileage.

Reviewer 2:

The reviewer noted that the project provides a deep understanding and guidance for the potentially high-energy systems.

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 there is quite a bit of work left in the project and the effort seems appropriately funded. However, the reviewer expressed a misunderstanding of why a 0.1 full-time equivalent (FTE) staff scientist and a 1.5 FTE postdoctoral scholar cost \$430,000 per year, even at a national laboratory.

Reviewer 2:

The reviewer noted that resources included that right blend of experts.

Energy Storage Materials Research Using DOE's User Facilities: Michael Thackeray (Argonne National Laboratory) - es235

Presenter

Jason Croy, Argonne National Laboratory.

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 approach of using multiple diagnostics techniques to understand the behavior of high-energy cathodes is excellent. The team uses high-resolution X-ray diffraction crystallography (XRD), neutron diffraction, XAS, electron microscopy and other techniques.

Reviewer 2:

The reviewer observed that the PIs used different characterization technologies to investigate the structure-property relationship.

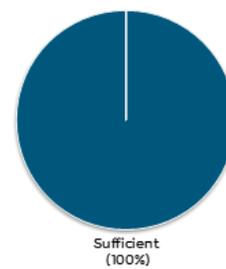
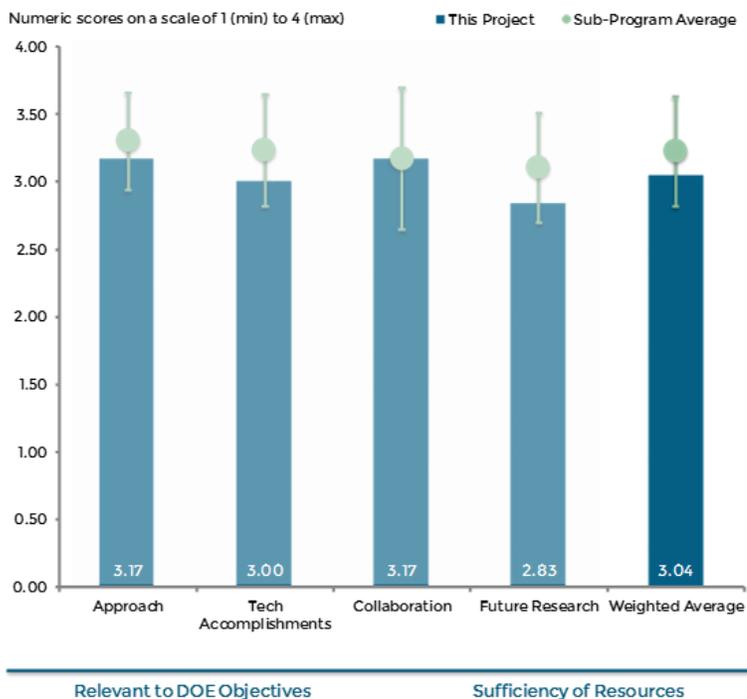
Reviewer 3:

The reviewer remarked that the characterization tests being conducted are sufficient to understand electrode design, and that it will be interesting to see if any of the models will be able to predict better structures. The reviewer is concerned about the titling of this project as a user facility. It does not appear there was a large number of users outside of ANL.

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 towards DOE goals.

Reviewer 1:

The reviewer stated that there have been significant characterization studies undertaken by this project and that on the whole, the PowerPoint was well done and the insights from the project were well communicated.



es235

Figure 2-52 Energy Storage Materials Research Using DOE's User Facilities: Michael Thackeray (Argonne National Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer reported that the results are good, but wondered if one could focus more on the issues that impede the layered/layered cathodes from reaching commercial acceptance (e.g., low SOC impedance, poor packing density, etc.). This comment is not solely focused on this project, but rather applies to many of the diagnostics efforts in the program.

Reviewer 3:

The reviewer observed that there was lack of coordination on different technologies for after few year study, no solid conclusions were made. Only that the design space is large and complex.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer commented that the project team has a very good list of collaborators.

Reviewer 2:

The reviewer said it is a team work.

Reviewer 3:

The reviewer said that while there is a significant number of collaborators, there is concern that there is no engagement of private sector companies. For reference, it would be helpful to also have some industry produced material standards.

Question 4: Has the project 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 PIs should focus on understanding the mechanism using different characterization technologies, and then design the electrode materials.

Reviewer 2:

The reviewer reported that as this project is nearly completed, there is some concern about the ability to accomplish the tasks laid out in future work. The reviewer expressed if this work is already underway and will it just be completed during the next quarter. The long term impact on electrode design considerations could be substantial after this work is completed, and it will require broader engagement of the research community.

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

Reviewer 1:

The reviewer said that the project's development of better cathodes either through material work or processing work, directly improves the performance of batteries. It is this that limits the performance.

Reviewer 2:

The reviewer noted that this work fits in with the DOE goal to reduce GHG 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 commented that project team's work is a good value for the budget, with excellent progress and data.

Reviewer 2:

The reviewer observed that the PIs have the resources to do the work.

Reviewer 3:

The reviewer noted that the funding is sufficient for this work.

Crash Propagation Simulations and Validation: Shriram Santhanagopalan (National Renewable Energy Laboratory) - es236

Presenter

Shriram Santhanagopalan, National Renewable Energy Laboratory.

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 stated that the approach is good and the modeling of the actual predicted cell deformation is anticipated to provide better failure mode identification capability. The reviewer posed the question whether an electro-chemical aspect to the multi-domain modeling should be considered.

Reviewer 2:

The reviewer noted that it is hard to see how the funds support the 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 towards DOE goals.

Reviewer 1:

The reviewer explained that the PIs have demonstrated the logic path moving from the mechanical deformation to the electro-thermal response, and have combined this with experimental validation to support the results.

Reviewer 2:

The reviewer commented that the technical accomplishments have been achieved as planned.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that the project team’s collaboration roles and effort appears to be well defined.

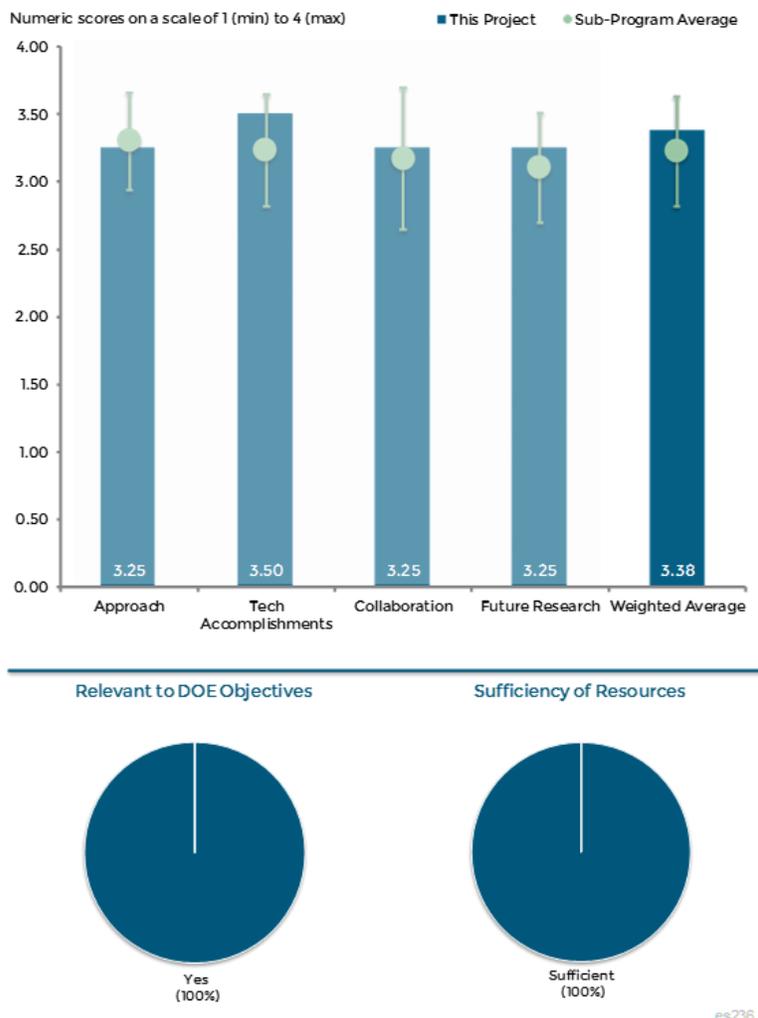


Figure 2-53 Crash Propagation Simulations and Validation: Shriram Santhanagopalan (National Renewable Energy Laboratory) - Electrochemical Energy Storage

Reviewer 2:

The reviewer inquired if it is possible to leverage the efforts of other projects to save the efforts in validation.

Question 4: Has the project 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 remarked that it might be a good idea to at least consider a framework for incorporating the electro-chemical aspect of the problem into the simulation platform. The reviewer asked if a full battery pack damage demonstration test will be considered as full validation of the approach.

Reviewer 2:

The reviewer asked if it is possible to include the study of the impact of battery management systems (BMS) and thermal system on the crash propagation in the future research.

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

Reviewer 1:

The reviewer stated that the development of predictive modeling capabilities for battery damage will enable the design of more damage-tolerant systems.

Reviewer 2:

The reviewer noted that the project predicts battery safety during crash and can potentially help the battery design.

XG Sciences: Development of Silicon Graphene Composite Anode: Robert Privette (XG Sciences) - es237

Presenter

Robert Privette, XG Sciences.

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 graphene and silicon composite will produce advanced anodes for Li-ion batteries and manufacturing process is being developed.

Reviewer 2:

The reviewer explained that it seems the two major components to this project are materials development and process scale development. Slide 11 shows a material and cell that meets the 500 cycle milestone goal, but Slide 12 shows a next generation technology that in regards to DOE, does not meet the goal even in the coin cell. The reviewer remarked that the path to both scale-up and cycle life is not clear, and is also not sure about the use of the term graphene platelets. If the plates are multi-layered, then they are graphite platelets. The reviewer added that 600 mAh/g is among the lowest energy densities of the anode projects at the AMR, and 1,000 cycles to 80% retention would be a better goal. Also, just as a reference the USABC goals for EV batteries are 350 Wh/kg useable at end-of-life (EOL) plus 1,000 cycles of the full usable range, and that 1,000 cycles at 80% depth-of-discharge (DoD) will probably fall a little short of this goal. This is a 2020 goal and while it may not be applicable to this stage of the research, it is good to keep in mind if the end goal is the automotive environment.

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 towards DOE goals.

Reviewer 1:

The reviewer stated that the composite anode capacity is validated with the newly developed coating process.

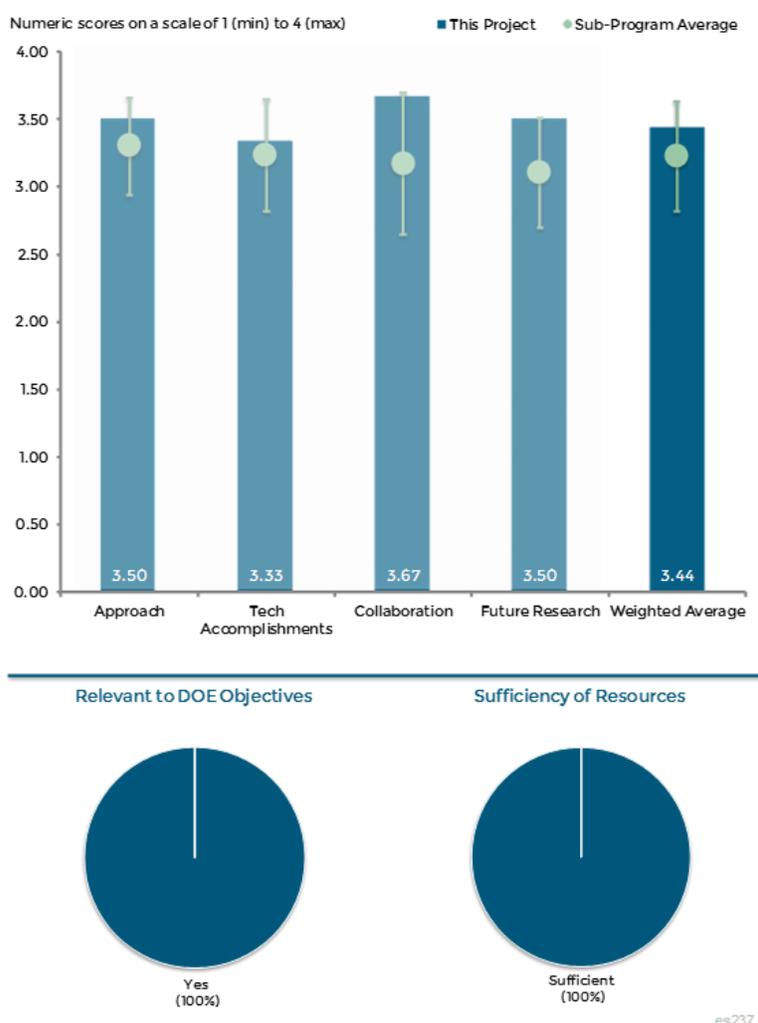


Figure 2-54 XG Sciences: Development of Silicon Graphene Composite Anode: Robert Privette (XG Sciences) - Electrochemical Energy Storage

Reviewer 2:

The reviewer said that in reference to above comments, though the GEN3 material is stable over a wider voltage range, the fact that it does not meet even the 500 cycles to 70% capacity retention, shows there are still significant technical barriers to overcome in this project. The reviewer expressed the need to see more information on the volumetric energy density of this material, as well as the rate capabilities.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer explained that the scale-up work at the A123 Systems and the ANL facility, is a big strength of this project.

Reviewer 2:

The reviewer noted that the involvement of high-volume global cell producer is the only area for possible improvement.

Reviewer 3:

The reviewer commented that the partners include the leading battery suppliers, component suppliers, and research laboratories.

Question 4: Has the project 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 future work will validate the manufacturing process and the cycle life.

Reviewer 2:

The reviewer commented that the project is on the right track, however, as mentioned in above comments there are still very significant technical challenges to overcome, and from the presentation slides, it is very difficult to see a path to doubling the cycle life of this material.

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

Reviewer 1:

The reviewer noted that the high-energy anode will help with the penetrations of the EV acceptance.

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

Reviewer 1:

The reviewer observed that the project seems worthy of greater resources.

Reviewer 2:

The reviewer stated that the money and resources seem sufficient.

Low-Cost, High-Capacity Lithium-Ion Batteries through Modified Surface and Microstructure: Pu Zhang (Navitas Systems) - es238

Presenter

Pu Zhang, Navitas Systems.

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 explained that the approach of macro-porous Si with controlled pore structure to accommodate the large Si volume internal change, is a good approach.

Reviewer 2:

The reviewer explained that on Slide 8, using coin cells as proof of technology is a good preliminary step, but may not prove that this material has greater cycle life than a non-porous Si anode in a full cell configuration. Also very little information is given about the composition of each anode, so it is hard to make a technology assessment from this slide. The reviewer added that as shown on Slide 5, HF may not be the best method to use for etching unless one can fully remove the HF before using the material, which is surely already known, for HF is well known for contributing to degradation in Li-ion cells. On Slide 3 and 4, mAh/cm² is a large coating. The reviewer expressed a need to be worried about the rate performance of these electrodes as not being good enough for the automotive environment. Also, just as a reference, the USABC goals for EV batteries are 350 Wh/kg useable at EOL plus 1,000 cycles of the full usable range, and that 1,000 cycles at 80% DoD will probably fall a little short of this goal. The reviewer went on to say that this is a 2020 goal, and while it may not be applicable to this stage of the research, it is good to keep in mind if one’s end goal is in the automotive environment.

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 towards DOE goals.

Reviewer 1:

The reviewer observed that GEN1 material has been developed with 800 mAh/g capacity and 15% initial capacity loss (ICL).

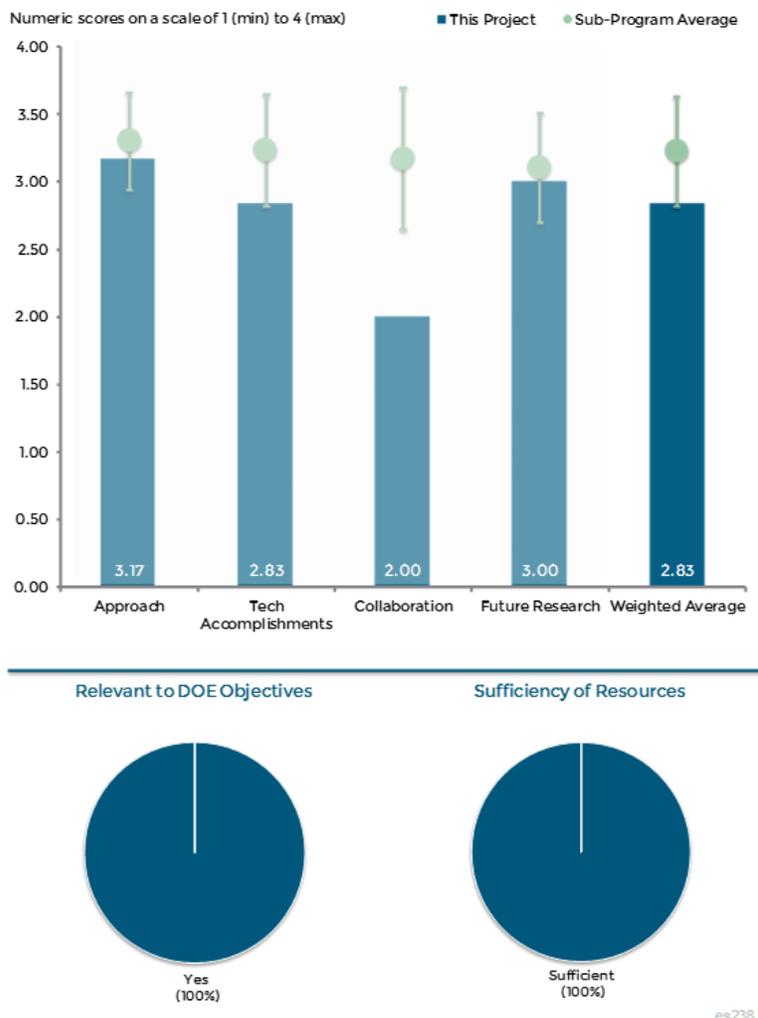


Figure 2-55 Low-Cost, High-Capacity Lithium-Ion Batteries through Modified Surface and Microstructure: Pu Zhang (Navitas Systems) - Electrochemical Energy Storage

Reviewer 2:

The reviewer commented that on Slide 6, cycle life seems to be a large issue in this project, and noted that data showing that the phase-1 cycle life of 300 cycles at 100 percent DoD was met, could not be seen. In general, the title of the project contains the words low-cost, but any information or goals pertaining to cost anywhere in the slides, could also not be seen.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that the planned collaboration with A123 Systems and Xalt Energy is satisfactory, but project team also needs high-energy cathode collaboration.

Reviewer 2:

The reviewer commented that all of the work is being done by Navitas Systems as far as far as the reviewer could tell, and suggested collaborating with other partners, particularly when it comes to the artificial SEI work.

Reviewer 3:

The reviewer explained that A123 Systems and Xalt Energy are listed as possible partners, but it is unclear how and if they can and will support this project, or if they would be appropriate at this stage of development.

Question 4: Has the project 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 pilot scale etching and SEI formation will help to validate the concept of using large format cells, and that the swelling of the cells needs to be monitored and with mitigation if necessary.

Reviewer 2:

The reviewer explained that on Slide 17, there was no mention in the project of improving cycle life, unless it is being alluded to by the SEI coating to improve the performance. Because there is no data in the project showing even 200 cycles to 80% capacity retention, the main focus of the future work has to be improving cycle life. The reviewer added that electrolyte may also play a large role in making this technology viable, but it is not mentioned at all in the future work.

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

Reviewer 1:

The reviewer said that the advanced anode and high-energy cathode will improve the probability of EV applications which will reduce petroleum usage.

Reviewer 2:

The reviewer commented that the concept is very promising, but there is still a lot of work to be done to make a viable material for commercial use.

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 funding resources that follow original proposal, is enough.

Scale-Up of Low-Cost Encapsulation Technologies for High-Capacity and High-Voltage Electrode Powders: David King (Pneumaticoat Technologies) - es239

Presenter

David King, Pneumaticoat Technologies.

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 reported that the ALD coating is beneficial to the stability of the anode and cathode in the electrolyte.

Reviewer 2:

The reviewer remarked that this is a very interesting project. Slide numbers would be helpful to the reviewers. In regards to the slide that shows ALD versus co-precipitation, this slide is hard to evaluate ALD 1 and ALD 2, and asked if these are the team’s scaled up ALD processes or represent a more standard ALD process. The reviewer commented that if these not the team’s scaled up ALD processes, then a test of the project’s semi-continuous ALD process versus a lab scale ALD process, would be an important comparison. Referring to the slide that shows pouch cell ALD performance, the bottom says demonstrated performance but the slide indicates the testing is only to approximately 250 cycles. In all, the reviewer expressed that the technology is very interesting, but as a reviewer, it can be difficult to understand the presentation. Labels indicating whether the ALD coating was a standard batch process or your semi-continuous process would be helpful in evaluating the 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 towards DOE goals.

Reviewer 1:

The reviewer noted that the project team’s down-select progress is appropriate.

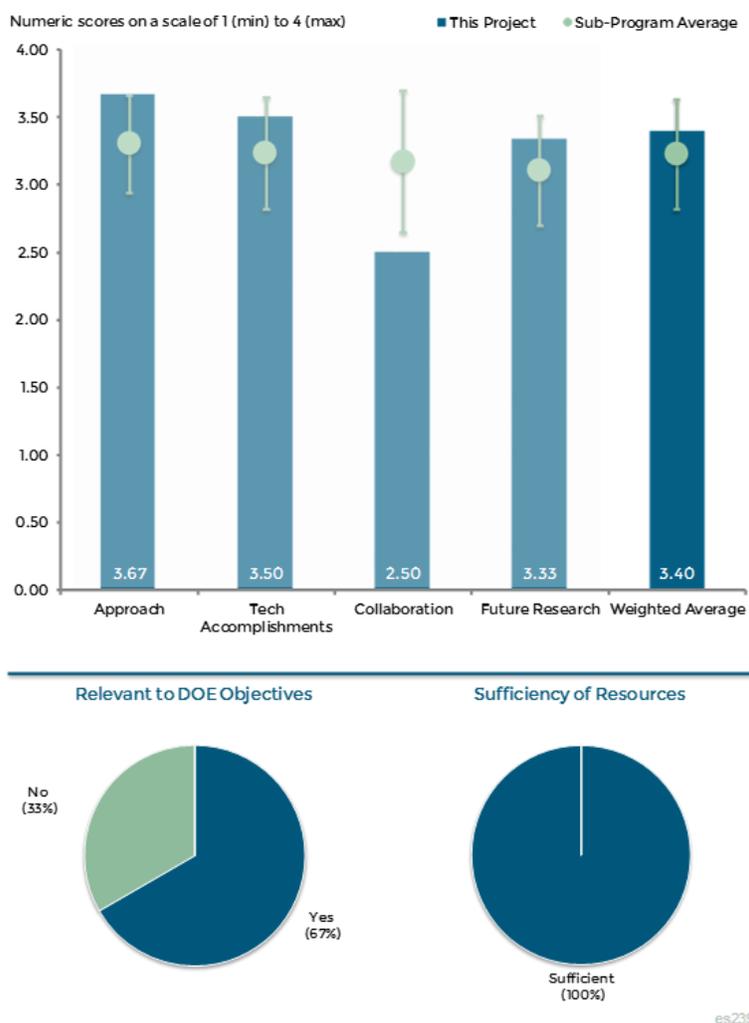


Figure 2-56 Scale-Up of Low-Cost Encapsulation Technologies for High-Capacity and High-Voltage Electrode Powders: David King (Pneumaticoat Technologies) - Electrochemical Energy Storage

Reviewer 2:

In reference to the above notes, the reviewer explained that it seems that a variety of materials have been tested, which is good, but this variety also confuses the ability to understand the progress of the technology. The data moves from NMC to LMR-NMC to LNMO/LTO, so it is hard to clearly see the progress from phase-1 to phase-2.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that the Xalt Energy collaboration will lead to improve the battery cycle life and performance.

Reviewer 2:

The reviewer stated that there is not a slide explicitly showing the collaboration with other institutions, but reading between the lines, it seems that good collaboration is taking place with materials suppliers and cell manufacturers.

Question 4: Has the project 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 a study with one material, or even two different materials and coatings, that show the cycle life of the uncoated material, the batch ALD coated material, the team's semi-continuous ALD coated material, and the ALD coated electrodes with all other things held constant, would be a good way to more clearly show the progress and viability of the research. More cost data would also help evaluate if the technology is economically viable.

Reviewer 2:

The reviewer stated that the planned system reliability and electrochemical reproducibility studies using 200 kg of cathode powders will provide the need for a quality coating for battery suppliers.

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

Reviewer 1:

The reviewer remarked that yes, the project supports the DOE goals, and if this technology is successful, it will be an excellent technology for coating electrode materials for mass production.

Reviewer 2:

The reviewer said that the improvement in cell longevity will provide the cost reduction per cycle and will help with 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 stated that project team has excellent progress considering budget size.

Reviewer 2:

The reviewer noted that the resources are good enough for coating studies.

Development of Silicon Graphene Composite Anode: Samir Mayekar (Sinode Systems) - es240

Presenter

Cary Hayner, Sinode Systems.

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 3D graphene structure will help with Si insertion to improve anode capability.

Reviewer 2:

In reference to Slide 3, the reviewer stated that an anode of 750 to approximately 1,500 mAh/g leading to a 200 Wh/kg cell in regards to DOE, does not seem quite right, for the cell goal should be closer to 300-350 Wh/kg. Also, just as a reference, the USABC goals for EV batteries are 350 Wh/kg useable at EOL plus 1,000 cycles of the full usable range, and that 1,000 cycles at 80% DoD will probably fall a little short of this goal. The reviewer added that this is a 2020 goal, and while it may not be applicable to this stage of the research, it is good to keep in mind if the end goal is the in the automotive environment. The reviewer went on to say that in Slide 5, the approach is very novel and quite interesting, but is not sure how the holey-graphene material is produced and if it is tailorable for holey-ness.

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 towards DOE goals.

Reviewer 1:

The reviewer remarked that the project team has outstanding work, particularly with the given budget.

Reviewer 2:

The reviewer commented that Slides 8 to 12 showed the various areas of focus, materials sourcing, composition, etc., leading to improvements in the cycle life of the material. However, there is still significant process to be made to reach the cycle life goal. In reference to Slide 14, some binding agent may be needed in

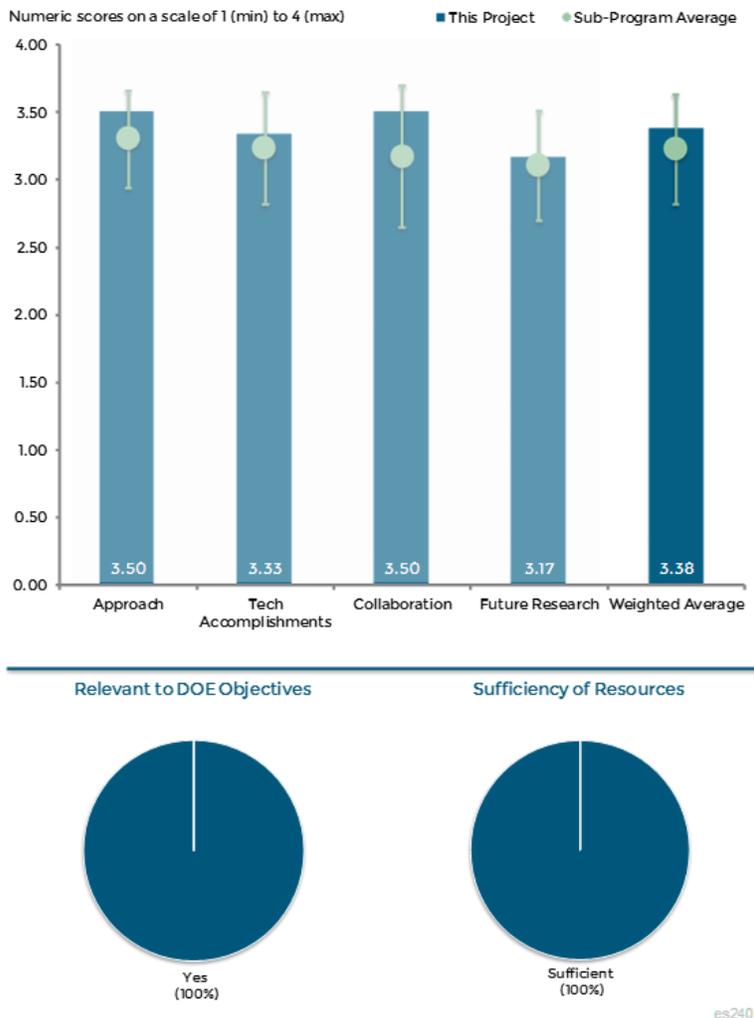


Figure 2-57 Development of Silicon Graphene Composite Anode: Samir Mayekar (Sinode Systems) - Electrochemical Energy Storage

order to keep the electrode attached to the current collector, where Slide 5 mentions that minimum inactive material is used in the anode formulation.

Reviewer 3:

The reviewer explained that the failure modes are identified and mitigation using coating, additives, etc., is planned.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that in Slides 10 and 11, the project team's collaborations with other institutions is good particularly in the area of materials analysis.

Reviewer 2:

The reviewer remarked that the project team has excellent collaboration and partners, where the only improvement could be to have involvement of a leading international cell manufacturer.

Reviewer 3:

The reviewer noted that collaboration with the university, material supplier, and the cell builder will expedite the development.

Question 4: Has the project 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 on Slide 17, the approach to the research is very good. The biggest challenge for this work to meet the DOE goals is to improve the cycle life, and that some more focus on methods to improve the cycle life should be included in this slide or else it is hard to see a path to meet these goals. Scale-up work is also very important and not covered in very much detail in the presentation. The reviewer added that while this is primarily an anode program, the goals are on the cell level, so some electrolyte work may be necessary in order to meet the goals.

Reviewer 2:

The reviewer noted that the failure modes are identified and the mitigation using coating additives, etc., is planned.

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

Reviewer 1:

The reviewer commented that the advanced anode will reduce the cost of the batteries and will help with electrification of automobiles.

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 the \$500,000 should be sufficient to meet the planned progress.

A Disruptive Concept for a Whole Family of New Battery Systems: Farshid Roumi (Parthian Energy) - es242

Presenter

Farshid Roumi, Parthian Energy.

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 Li wire anode and Si anode's hybrid concept may be an acceptable approach.

Reviewer 2:

The reviewer commented that this work is in its preliminary stages, so it is difficult to review. In reference to Slide 3, 450 Wh/kg is a very aggressive goal, however, 500 cycles is not, plus there is no capacity retention specified. The reviewer expressed that a reasonable goal should be more like 700-800 cycles at 80% DoD to 80% capacity retention.

If there is no path to do this, then scalable fabrication would be a waste. The reviewer also expressed a need to see a goal in terms of Wh/liter (L). In reference to Slide 5, the photos are not showing a fabrication method.

Reviewer 3:

The reviewer asked if the current collection of designs is for anode or cathode, separator tube fabrication, current distribution in cathode plate, and electrolyte retention and distribution.

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 towards DOE goals.

Reviewer 1:

The reviewer commented that in Slide 7, more information is needed on this slide, and asked where the cycle method and rate was, and if this is really a copper-LiCoO₂ cell or is Cu the current collector. There is a large gap to fill in terms of cycle life in this project. The reviewer also asked how the team will know if this technology will cycle, and what the plan is for a separator. In Slide 9, there is no proof of concept in this photo. The reviewer asked for data. The reviewer also questioned the schedule on Slide 12, where it is hard to

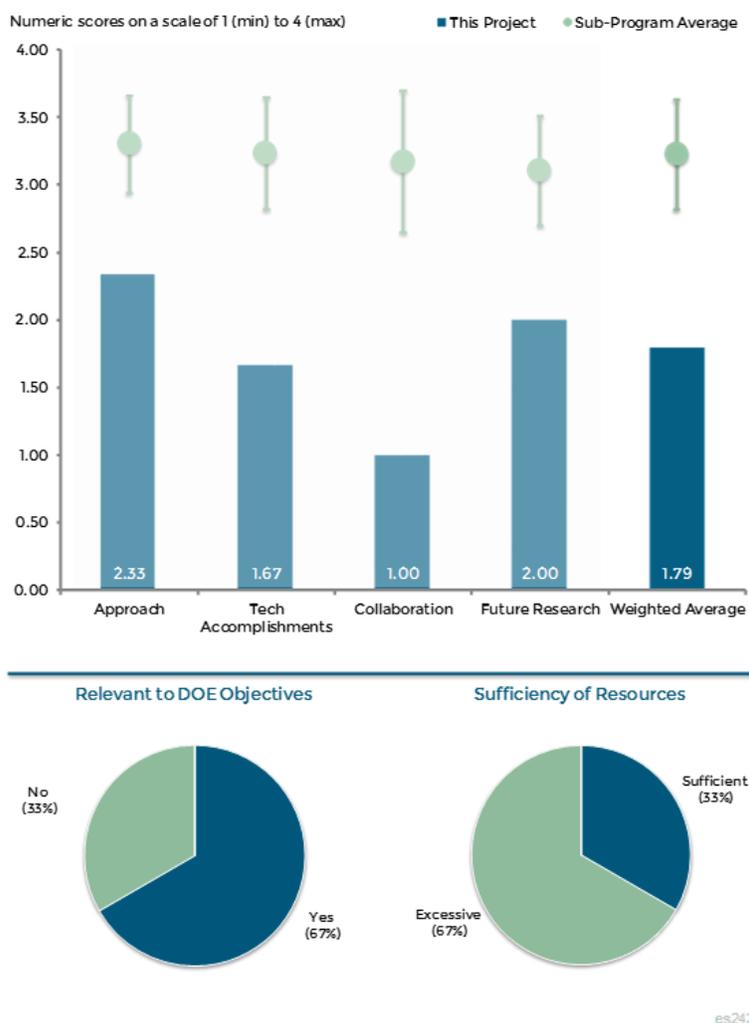


Figure 2-58 A Disruptive Concept for a Whole Family of New Battery Systems: Farshid Roumi (Parthian Energy) - Electrochemical Energy Storage

evaluate the state of the research without knowing where to look in the deliverables schedule, and where the referenced 5 Wh cells fit into the deliverables.

Reviewer 2:

The reviewer noted that the demonstration of the concept with a cathode is not shown.

Reviewer 3:

The reviewer remarked that the project's progress is either poor or there is not enough detail to judge.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that there is no collaboration with a cell manufacturer.

Reviewer 2:

The reviewer observed that no evidence of project team's collaboration is given.

Reviewer 3:

The reviewer noted that the project team's collaboration is either none or unknown.

Question 4: Has the project 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 it was very difficult to determine the project team's future research.

Reviewer 2:

The reviewer pointed out that in Slide 13, a 50-mile PHEV needs about 14.5 kWh of usable energy with approximately 95% to 25% SOC, which means that the actual cell needs to be about 30% larger. The reviewer expressed a need to know what the power capability of this cell is, and if it is 100kW as needed for a PHEV. Cycle life is a major concern, and there is not a clear path in the future work toward improving the cycle life.

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

Reviewer 1:

The reviewer stated that if successful, this project could be a high-reward program. However, there are many risks and challenges which are not well represented in this presentation.

Reviewer 2:

The reviewer commented that it was not made very clear how the cost of the cells and energy is improved.

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

Reviewer 1:

The reviewer observed that it seems this project is more like a science experiment in a lab and, therefore, may not need \$75,000.

Dramatically Improve the Safety Performance of Lithium-Ion Battery Separators and Reduce the Manufacturing Cost using Ultraviolet Curing and High Precision Coating Technologies:
 John Arnold (Miltec UV International) - es243

Presenter

John Arnold, Miltec UV International.

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 this approach is very interesting and relevant technology, and expressed a need to see more information about the resultant separator. See USABC separator goals as an example of important properties.

Reviewer 2:

The reviewer stated that any ceramic coating will improve the high-temperature stability of Li-ion separators.

Reviewer 3:

The reviewer explained that it is difficult to discern how this specific approach compares in terms of performance of benefits and disadvantages to other ceramic separator coating methods. The comparison of shrinkage of base film of a given thickness, to coated form of same given thickness base film with additional thickness from the included coating, seems inappropriate. The reviewer also noted that the ceramic coated base film that is patterned or otherwise, shows less shrinkage than the same uncoated base film, and this hardly seems like an advancement over the state of the art. The reviewer expressed a need to understand where the result is of a simple electrochemical stability analysis performed on just a small sample of the coated separator which is coated at the noted line speeds. The ability to coat patterns in transverse direction (TD) or machine direction (MD) coating and effect on shrinkage in TD or MD coating should be the major highlighted benefit if the potential stability issues with UV package could be assumed to be negligible.

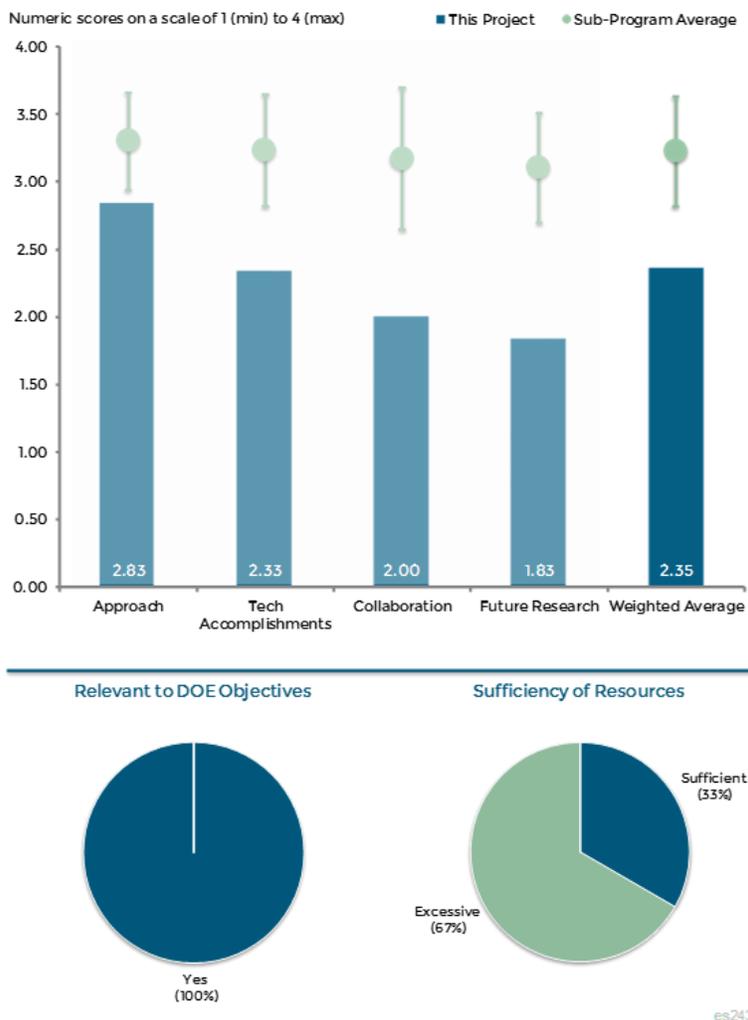


Figure 2-59 Dramatically Improve the Safety Performance of Lithium-Ion Battery Separators and Reduce the Manufacturing Cost using Ultraviolet Curing and High Precision Coating Technologies: John Arnold (Miltec UV International) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer explained that the shrinkage at 150°C should be less than 5% for an effective internal short prevention.

Reviewer 2:

The reviewer commented that just for the future, slide numbers make it easier to give clear comments. Regarding the slide entitled “Why ceramic coated separators?”, the reviewer inquired if the project team is sure increasing the ion path tortuosity is really a plus. High-voltage stability is a good goal, but there no evidence of this is in the presentation, nor does the reviewer see any plans to test for it. In reference to the slide “Novel Printed Patterns,” the reviewer said that this is interesting, but is not sure it is a good use of resources with so many fundamental questions unanswered. The reviewer would focus on whether the team’s material can meet the state of the art, or the USABC goals, before working on patterns. In reference to the slide UV ceramic coating on tri-layer, the slide has no meaning without a control, and also, 50 cycles are not enough. The reviewer asked how the project team knows the integrity of the coating is good. In reference to the slide shut down pattern, the reviewer asked if the electrochemical stability of the team’s shutdown coating is cycle life data or rate data of separators coated with the shutdown coating. In general, the process cost is missing, which is an important part of this work.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that it should be good that a major separator manufacturer is involved.

Reviewer 2:

The reviewer commented that based on the cover page, one can assume some project collaboration is taking place, but no information is given in the slides.

Question 4: Has the project 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 as mentioned above, there are still many unanswered questions about this technology which are not addressed in the presentation. In fact, there is not a slide addressing the future work at all, except on the slide with high-level milestones. The reviewer would like to see a lot more information about the properties of the separator or plans for testing the properties, if it has not been done yet.

Reviewer 2:

The reviewer said that the project has limited and ambiguous info regarding future research plan.

Reviewer 3:

The reviewer stated no clear path to improve high temperature shrinkage is identified.

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

Reviewer 1:

The reviewer stated that the safety of cells will improve the probability of using the cells for an automotive application.

Reviewer 2:

The reviewer remarked that this coating method has a potential to decrease the cost of coating separators, but there are currently many unanswered questions in the 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 reported that \$2 million for the separator coating is excessive and that the coated separators are available in domestic market.

Low-Cost, High-Capacity Non-Intercalation Chemistry Automotive Cells: Alex Jacobs (Sila Nanotechnologies) - es244

Presenter

Alex Jacobs, Sila Nanotechnologies.

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 the core-shell silicon-based anode versus core-shell metal fluoride (MF_x) cathode may have long life.

Reviewer 2:

The reviewer commented that this research is based on a sound concept that uses core-shell technology with a well-designed protective shell. However, due to proprietary considerations, very little information is provided on the specific technical approach in regards to chemistry and material science, and therefore, it is difficult to assess the technical approach.

Reviewer 3:

The reviewer stated that due to the limited information in slides and presentation, it was hard to evaluate technical approach.

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 towards DOE goals.

Reviewer 1:

The reviewer explained that half-cell performance is good enough for further development, and that the cell level cycle life should be greater than 1,000 cycles.

Reviewer 2:

The reviewer commented that in the approach, rate capability also must be demonstrated.

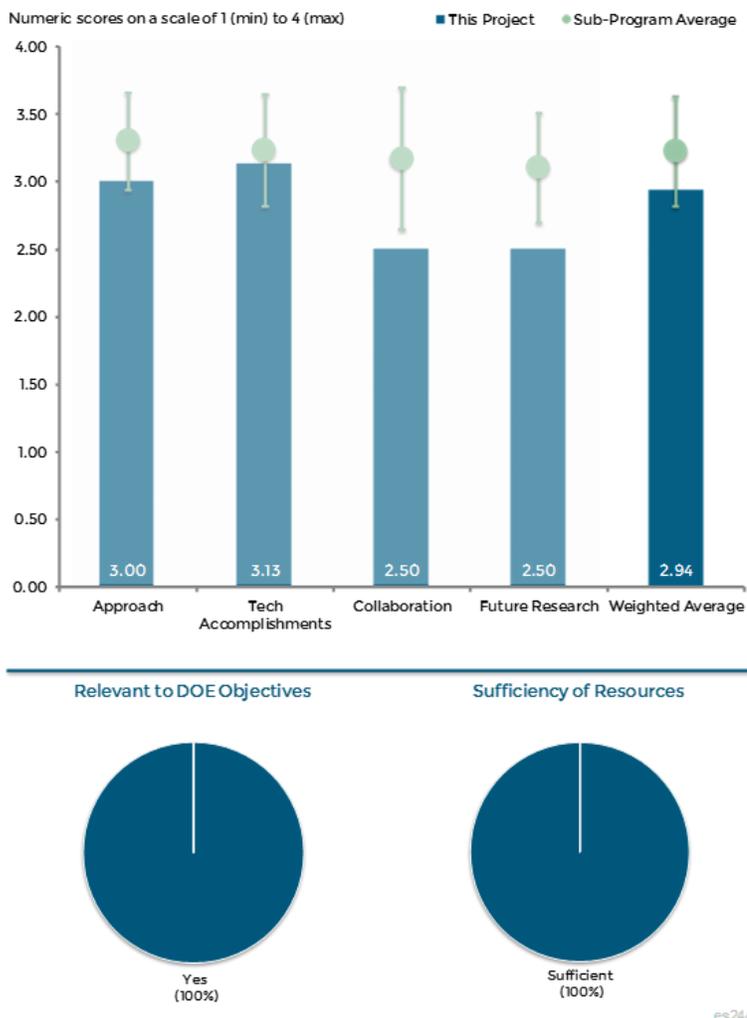


Figure 2-60 Low-Cost, High-Capacity Non-Intercalation Chemistry Automotive Cells: Alex Jacobs (Sila Nanotechnologies) - Electrochemical Energy Storage

Reviewer 3:

The reviewer stated that the results presented are promising, however, the electrode loading data is not provided.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer observed that project's collaboration partners are well established.

Reviewer 2:

The reviewer explained that collaboration partners would otherwise seem excellent, but the unknown automotive partner is not identified. It seems inappropriate to not identify a partner if they are generically highlighted.

Reviewer 3:

The reviewer stated that in addition to ARL and Georgia Institute of Technology, a cell developer must be included for further development.

Reviewer 4:

The reviewer remarked that it is not very clear in the project's collaboration of how the outcome from each institution is integrated.

Question 4: Has the project 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 it is important to plan technology demonstration with a full cell with a relevant capacity of 5 Ah or more.

Reviewer 2:

The reviewer commented that it is not very clear how the cells will be fabricated and the objectives will be validated.

Reviewer 3:

The reviewer noted that no future work is provided.

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

Reviewer 1:

The reviewer explained that the end goals of the project of 1,200 Wh/L and 580 Wh/kg are very impressive and should reduce the battery mass and volume significantly.

Reviewer 2:

The reviewer observed that the project supports increasing energy density for an automotive application.

Reviewer 3:

The reviewer stated that low-cost and high-capacity automotive cells are required to achieve the DOE plan.

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 \$1 million is sufficient.

Low-Cost, Structurally Advanced Novel Electrode and Cell Manufacturing: Taison Tan (24M Technologies) - es245

Presenter

Taison Tan, 24M Technologies.

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:

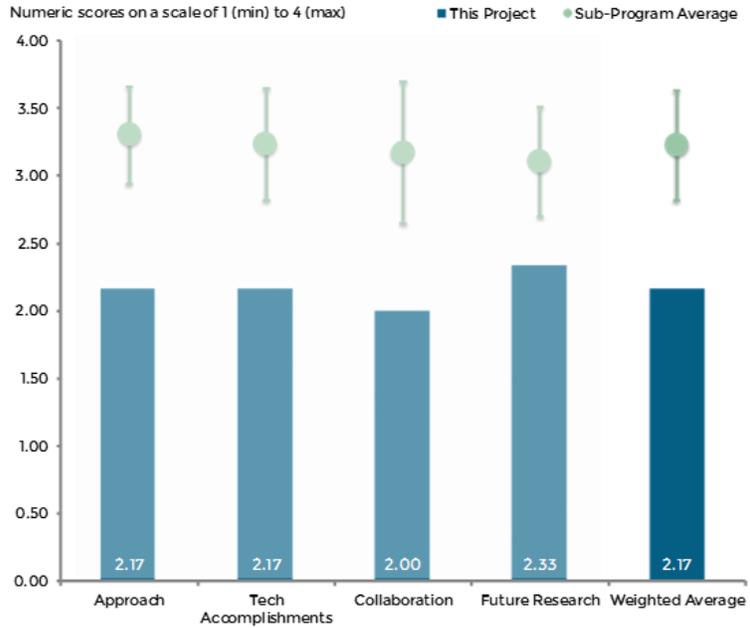
The reviewer said that using a new architecture to produce thicker electrodes for higher specific energy cell is a new approach.

Reviewer 2:

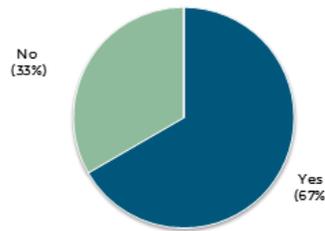
The reviewer commented that the project approach is unknown.

Reviewer 3:

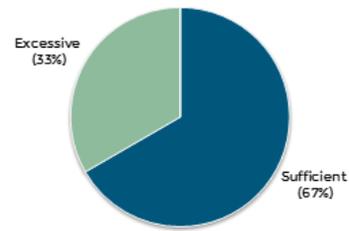
The reviewer expressed that the project approach is very difficult to assess given the paucity of information.



Relevant to DOE Objectives



Sufficiency of Resources



es245

Figure 2-61 Low-Cost, Structurally Advanced Novel Electrode and Cell Manufacturing: Taison Tan (24M Technologies) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer that the specific charge and discharge power looks good for a thick electrode.

Reviewer 2:

The reviewer stated that project team’s progress is unknown.

Reviewer 3:

The reviewer stated that there needs to be more information to assess the technical accomplishments. There is no cycling data, neither Wh/kg nor Wh/L.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team’s collaboration with equipment producers is good enough.

Reviewer 2:

The reviewer observed that the project has no partners, although perhaps that is appropriate given where 24M is in the development cycle.

Question 4: Has the project 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 development to increase the electrode thickness to meet high-specific energy goal is very important.

Reviewer 2:

The reviewer stated that the proposed future research is unknown.

Reviewer 3:

The reviewer remarked that the proposed future research has very few details, and cannot understand what issues the project team is having when trying to mitigate.

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

Reviewer 1:

The reviewer noted that the high specific energy cells will improve the probability of success.

Reviewer 2:

The reviewer stated that the project relevance is unknown.

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 \$2 million to prove the concept and cell development is sufficient.

Reviewer 2:

The reviewer observed that the project activity relative to resources is unknown.

Advanced Drying Process for Lower Manufacturing Cost of Electrodes: Iftikhar Ahmad (Lambda Technologies) - es246

Presenter

Iftikhar Ahmad, Lambda Technologies.

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 project's general approach seems excellent. Apparent oven design capabilities seem a little limited, and maybe, could have/could benefit from expertise or manpower of related normal oven equipment designers, but given the limits of the total budget situation which is understandable and the honest depiction of the actual current situation which is refreshing.

Reviewer 2:

The reviewer stated that the project team has sound approach and plan in demonstrating the technical feasibility of this technology.

Reviewer 3:

The reviewer noted that the approach is a drying process that uses microwave to reduce the drying time and the cost of drying.

Reviewer 4:

The reviewer remarked that the idea is quite straight forward, as many experimental studies on the effect of advanced drying process (ADP) on battery performance such as surface reaction and mechanical stability must be conducted. The cost analysis for drying process will also be needed in terms of energy and additional facility needed.

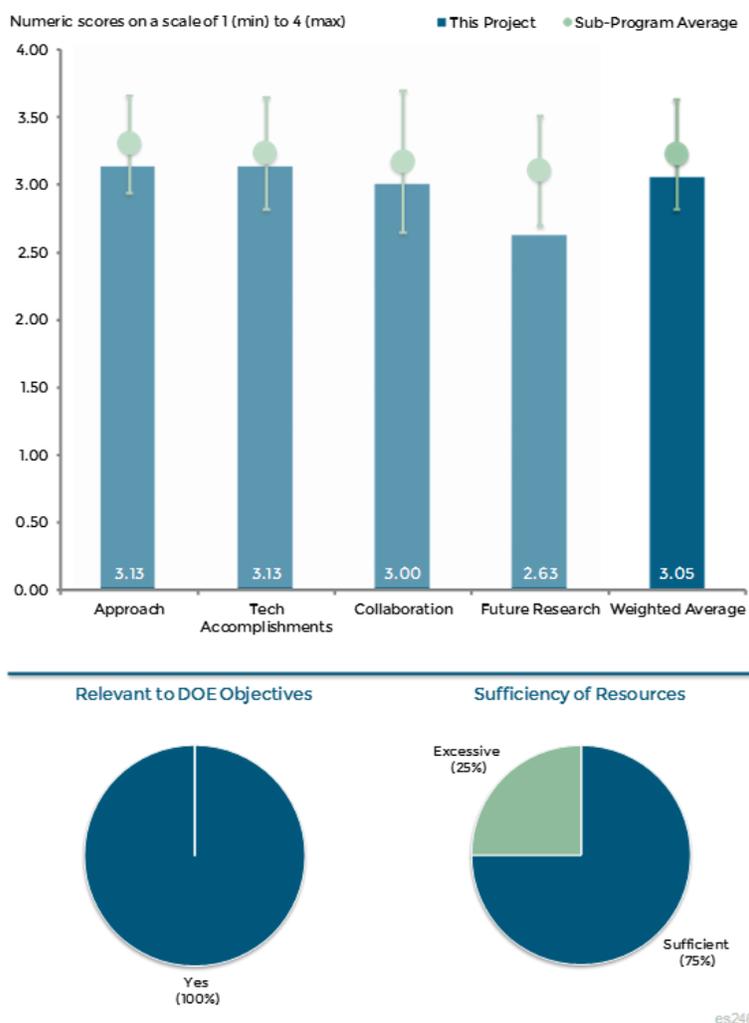


Figure 2-62 Advanced Drying Process for Lower Manufacturing Cost of Electrodes: Iftikhar Ahmad (Lambda Technologies) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer said that the comparison of drying time between standard and ADP methods was done under only one loading for anode and cathode, and it is useful to demonstrate the effect of loading on the drying time so that the work can establish the loading window in which the proposed ADP will be preferred over the standard method. The reviewer asked how the performance of drying time varies with anode type, specifically when comparing graphite and silicon-based anodes.

Reviewer 2:

The reviewer noted that the electrode samples had 2,000 parts per million (ppm) solvents.

Reviewer 3:

The reviewer remarked that adhesion and binder distribution tests are not clear about how they were conducted. Optimizing the proposed approach may further improve the outcome further. The reviewer also remarked that scalability would be of interest for practical purpose. Additionally, applicability for other materials will be important.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer said that Navitas Systems seems like a good and very appropriate partner for this project.

Reviewer 2:

The reviewer stated that the project team's collaboration with Navitas Systems seems to be well established, and the actual collaborative work is planned for the remainder of the project.

Reviewer 3:

The reviewer noted that Navitas Systems will evaluate the electrodes.

Reviewer 4:

The reviewer remarked that the project team's collaboration is not clearly described. A more detailed electrochemical test may be expected from the battery company collaborator.

Question 4: Has the project 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 continuation of collaboration with Navitas Systems will help.

Reviewer 2:

The reviewer stated that understanding final cell or electrode size limits, which is expected at end of project, would be useful.

Reviewer 3:

The reviewer commented that a safety test also must be conducted.

Reviewer 4:

The reviewer reported that a stated project goal is 30 to 50% cost savings, but the proposed work does not include a cost analysis. Cost comparison with conventional drying technology is essential in evaluating the

benefits of the ADP. The reviewer said that the potential safety issues related to the use of microwaves needs to be addressed.

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

Reviewer 1:

The reviewer noted that if the project team is successful, the cost of cell manufacturing will go down.

Reviewer 2:

The reviewer stated that this project aims to reduce the battery cost.

Reviewer 3:

The reviewer explained that cost reduction of manufacturing is necessary for the achievement of DOE's 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 expressed that the project seems worthy of additional resources, particularly if added expertise in normal Li-ion oven design is included.

Reviewer 2:

The reviewer commented that the detailed budget plan and its usage are not provided.

Reviewer 3:

The reviewer noted that \$1 million to develop the drying process may be excessive.

**EV Battery Development:
Herman Lopez (Envia Systems) -
es247**

Presenter

Herman Lopez, Envia Systems.

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 explained that the approach adopted in this project is systematic and well planned, and according to the information provided, the project execution follows the planning. Capacities and capabilities of the partners appear to be appropriately chosen. The reviewer opined that the barriers described on the poster are not barriers, but goals. Nevertheless, the goals to be achieved are ambitious, which are achieving USABC cell targets including cell energy and power goals, calendar and cycle life goals, and cost.

Reviewer 2:

The reviewer stated that the project has a broad scope covering multiple areas requiring improved materials, but has done an outstanding job of organizing the many aspects of the project work and identifying the key barriers to be overcome.

Reviewer 3:

The reviewer explained that the approach for testing new materials and identifying the best performing materials is reasonable, and the flow chart is helpful. Although it is hard to know, however, the reviewer expressed a need to know if it is better first to optimize electrodes, and then look for electrolytes, for example, if another set of electrodes could be better performing if a different original electrolyte had been chosen. The roadmap presented could lead to a local maximum in performance, preventing the group from reaching the overall maximum.

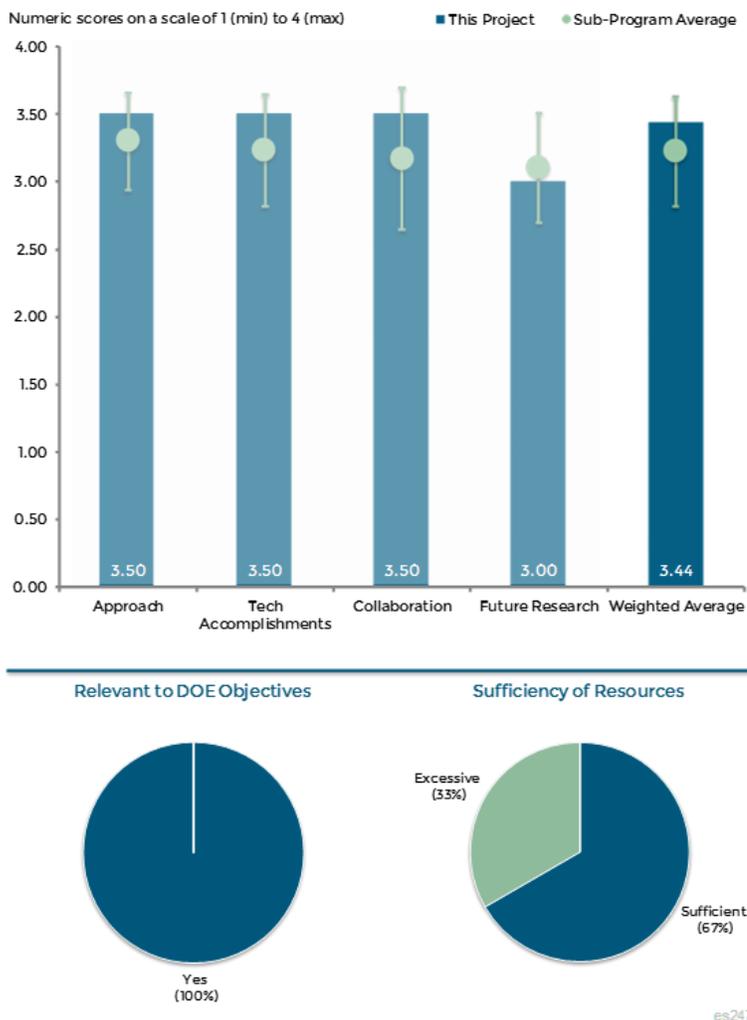


Figure 2-63 EV Battery Development: Herman Lopez (Envia Systems) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer commented that the technical work done has been considerable and matches the work plan of carefully selecting candidate materials for the next stages of the project.

Reviewer 2:

The reviewer observed that despite the incipient nature of the project of 25% completion, good progress has been demonstrated. The project is coordinated well with well-defined contributions from each partner combined with independent testing from Idaho National Laboratory (INL). The reviewer added that while the cycle life goal is 1,000 cycles, data on capacity fade has not been demonstrated above 200 cycles.

Reviewer 3:

The reviewer expressed an interest in the Si alloy materials composition and was told it was proprietary. It is hard to evaluate the practicality of a material without knowing its composition. Same comment about Asahi Kasei Corporation. Knowing the materials composition would be helpful in an evaluation, at least knowing if it is a polymer or ceramic at minimum. The reviewer asked if reviewers are to assume that if the company is interested in testing the separators, that they are thus cost effective enough to be commercializable. The reviewer asked what happens if they are not scalable. The reviewer also expressed that an evaluation cannot be provided without being able to learn more about the materials, and the same applies with the electrolyte.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the role of each partner is clear and the coordination of the execution of the work by the project leader appears good. Involvement and independent testing by INL is commended.

Reviewer 2:

The reviewer said that the project has many top industrial and national laboratory partners to provide expertise in the selected areas. The work done shows that these institutions have been well involved in the experimental work.

Reviewer 3:

The reviewer observed that there is a lot of coordination with companies, but it appears that no national laboratories or universities have been included. Some national laboratories were listed as part of the deliverables bullet, but without co-funding, the reviewer asked how they will guarantee their involvement.

Question 4: Has the project 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 project is still at an early stage but the timely achievement of milestones is encouraging, where the future work seems to be planned appropriately. More detailed information on a risk assessment exercise for a project would be useful to evaluate this criterion better, for example, how does this project evaluate the risk of a partner not delivering a material and component and what mitigating actions and alternatives are taken in this case to reduce the negative impact on the project outcome.

Reviewer 2:

The reviewer commented that the ambitious scope of the project has multiple barriers, especially in the silicon anode area. As such, it would be advisable to include some focus on searching out and evaluating new materials and technologies from others, such as prelithiation technology and ceramic separators.

Reviewer 3:

The reviewer noted that not many details about the future research were provided.

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

Reviewer 1:

The reviewer stated that higher performance batteries are a necessity to facilitate the displacement of petroleum in automotive applications by providing e-mobility options with performances meeting the consumer's expectations. This project has the potential to contribute to improving performance characteristics of LIBs.

Reviewer 2:

The reviewer said that the project is directed at the next generation, low-cost Li-ion battery for vehicles and thus fits in with the DOE's objectives.

Reviewer 3:

The reviewer noted that project probably supports the DOE's goals assuming that the materials being tested are scalable and cost-effective.

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

Reviewer 1:

The reviewer observed that the large number of partner institutions provide sufficient resources when combined with the resources at Envia Systems.

Reviewer 2:

The reviewer expressed that resources should not be directed to projects for which materials composition is not revealed, and to understand if other researchers are supposed to benefit when the results are proprietary materials. Only the companies benefit in this case.

Development of a PHEV Battery: John Busbee (Xerion Advanced Battery Corporation) - es248

Presenter

John Busbee, Xerion Advanced Battery Corporation.

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 project milestones appear to be on track, and the approach to compare the performance with commercial cells is commended as is the independent testing by ANL. The technical accomplishments are well documented and evidenced with data.

Reviewer 2:

The reviewer observed that no representative of Xerion Advanced Battery Corporation was at their poster for all or nearly all of the session, so it was not possible to ask questions to clarify aspects of the project. The manganese oxide spinels (LMO) cathode design and process appears to be very complex, for it is difficult to see how this could provide a low-cost LMO cathode with consistent quality. The reviewer went on to say that the pores are described as Nano-scale, but the SEM photos of the pores appear to be about 1 micron in size, not the 0.1 micron or less diameter of nano-scale. In the approach, there was no discussion of the percent porosity of the LMO cathode of this project as compared to the about 30% porosity of the calendared LMO cathodes now being used. The reviewer stated that a large focus of this project is on high-power rates, but this is only valid if the percent porosity of the LMO cathodes of this project is not well above the about 30%.

Reviewer 3:

The reviewer commented that while work is definitely an interesting technology, the reviewer would like to know how scalable the scope is, what the current cost is, and does the foam contains both the Li metal oxide and conductive carbon, or another composition. The reviewer also expressed to know how much sacrificial material is lost during the electrode fabrication process, how much is this cost, if it is isolatable after removal, and if these cathodes have ever been tested in full cells. The reviewer noted that it would have been good to ask the PI these questions, but no one was at the poster during the poster session, and the reviewer checked multiple times.

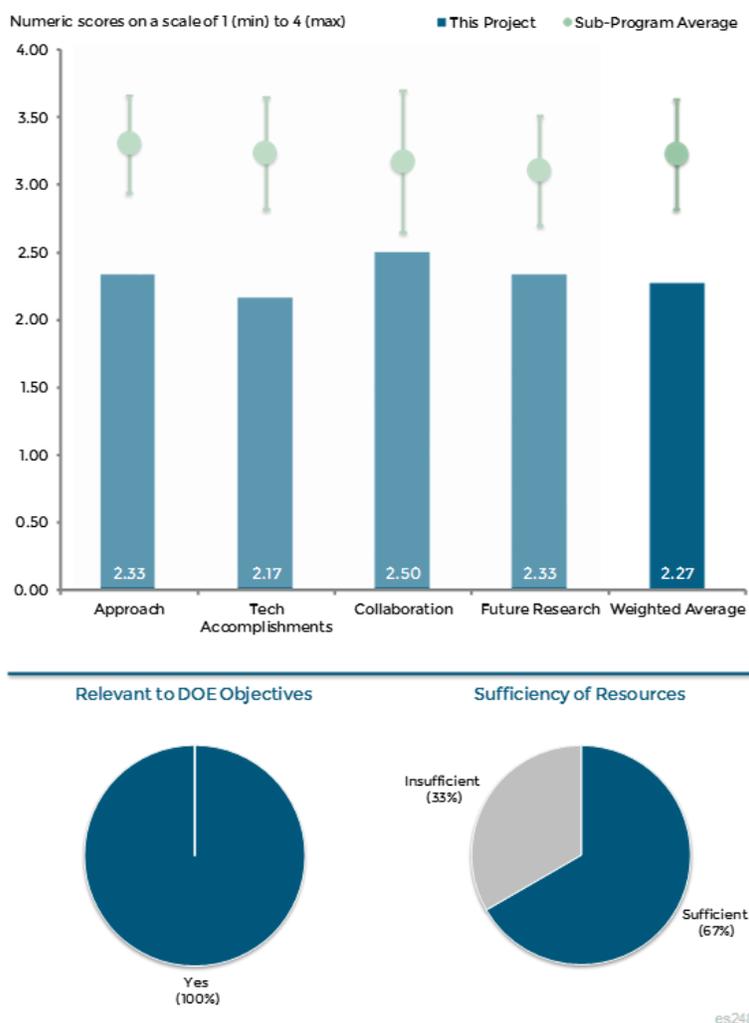


Figure 2-64 Development of a PHEV Battery: John Busbee (Xerion Advanced Battery Corporation) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer stated that in general, the technical accomplishments are well described. The specific energy claimed of 260 Wh/kg, is based on electrode weight; however, its specific energy relative to cell weight as per the USABC target cannot be evaluated.

Reviewer 2:

The reviewer asked why the LMO was selected over LCO in October 2014, and where the cycling data is showing that both materials were made and studied, or if only LMO was fabricated. The reviewer also asked on what scale the electrodes have been fabricated, and how many batteries have been fabricated and tested. The reviewer commented this product should be tested side-by-side with commercial cathodes, not pulling data from the literature and at different charging rates.

Reviewer 3:

The reviewer remarked that it is hard to evaluate the LMO cathodes of this project without having controls of conventional LMO cathodes, and without having some full cell data on at least the small cells. This project appears to be set up to compare the new LMO cathodes directly with typical LMO cathodes and to evaluate the new LMO cathodes, but it is not clear whether this was done, and what the anode, separator, and electrolyte each was used in the cells.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer observed that some partners and collaborations are mentioned. However, there is no information on what their contributions were and how they were coordinated.

Reviewer 2:

The reviewer explained that there is some project team collaboration with other institutions, but it is not clear what work that the team has done on the project.

Reviewer 3:

The reviewer commented that it is unclear what the coordinated activities with the institutions listed have been or will be. For example, the reviewer asked if the University of Illinois at Urbana-Champaign (UIUC) is getting funding to help with microstructural characterization, and what kind of testing has Intertek done or will do. The reviewer asked does the current award support these collaborators, but if not, how will collaborators make a significant contribution to the project.

Question 4: Has the project 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 is approaching its conclusion in October 2015. Progress to date has been good, however, there are a number of outstanding barriers and challenges, and the time remaining also seems very short to achieve these objectives. As a general comment, the pdf of this poster was only available at the last minute. The poster was not hanging in the poster session, nor was anyone present. This has made the review of this work more difficult and the reviewer is not completely confident with some of the comments made. There are many things that the reviewer would have liked the PI to clarify during the poster session, but this was not possible.

Reviewer 2:

The reviewer noted that at this point in the project, the remaining barriers are not well characterized in terms of performance gaps and process feasibility, quality, and cost. Having the future research merely indicate building larger and more cells does not identify the barriers remaining and how they will be overcome.

Reviewer 3:

The reviewer observed that it appears that a lot remains to be done to determine if the material has a chance for commercialization. Specifics are not provided, and the PI was not available to answer questions about future tests, and therefore, a low score is being assigned due to lack of information.

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

Reviewer 1:

The reviewer commented that the project is directed at one aspect of improving Li-ion batteries by making the next generation cathodes.

Reviewer 2:

The reviewer commented although this research is in much more basic stages than what would have been expected.

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 number of likely barriers to prove the feasibility of a new approach to LMO cathodes that involves many process steps and new current collection technology, combined with the relatively small budget of the project, appear to be insufficiently resourced.

Reviewer 2:

The reviewer noted that there is not enough information to judge if the resources are adequate or not.

Battery Development: Mohamed Alamgir (LG Chem Power, Inc.) - es249

Presenter

Mohamed Alamgir, LG Chem Power, Inc.

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 project is taking a broad approach to overcoming the cold-cranking barrier starting with cathode materials and porosity and then evaluating the anode, electrolyte, and separator materials. The project has a good strategy to meet the low-cost pack barrier.

Reviewer 2:

The reviewer reported that the barriers being addressed in this project are clearly identified and the approach adopted is logical to try to overcome these barriers. Cost and performance at low-temperature are clearly critical barriers in this specific application, and addressing cost through simplifying the BMS is the correct approach. The reviewer went on to comment that the use of the term Polymer in the title of the project's poster of the 12V Start-Stop Li-Polymer Battery Pack is confusing, if not misleading, for a system that uses a non-aqueous electrolyte.

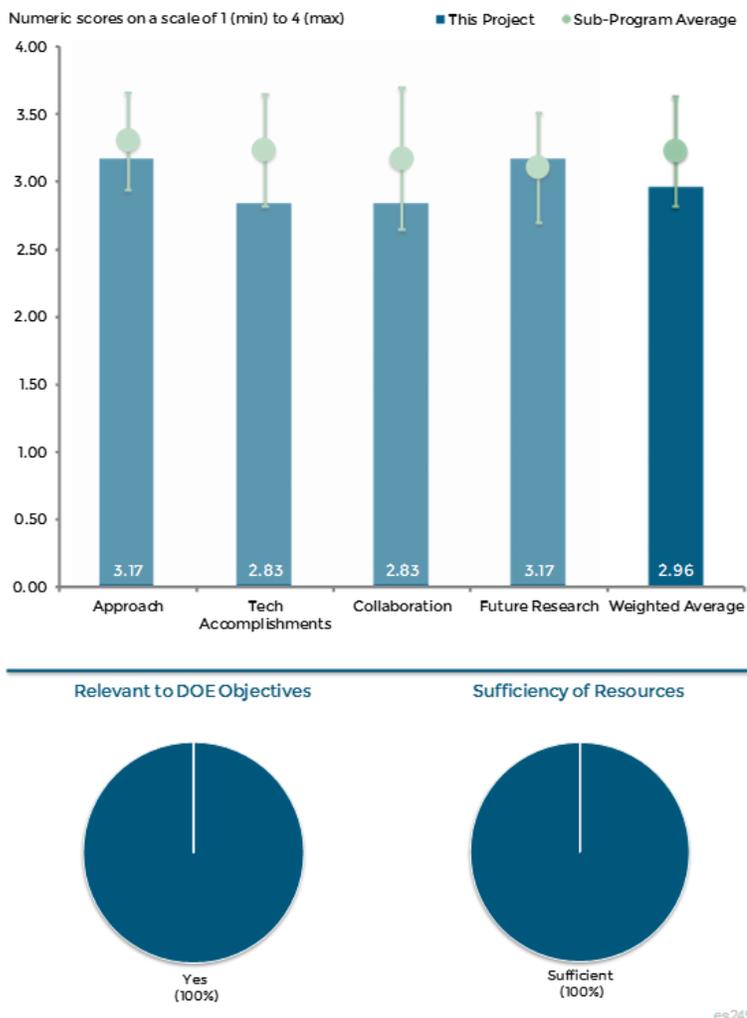
Reviewer 3:

The reviewer noted the bullet point lower cost close to the \$220 target, and asked what does this mean, and how close is the project to the team's actual goal. While the PIs are clearly doing work to improve performance, the approach is vaguely 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 towards DOE goals.

Reviewer 1:

The reviewer commented that the project work on the cathodes was useful as the first step in achieving the cold-cranking performance. Some quick screening of candidates for the anode, electrolyte, and separator would



be good to see if one or more of these materials has good potential for further optimization to overcome the low-temperature performance gap.

Reviewer 2:

The reviewer observed that this project only started at the end of last year, and it is difficult to judge the achievement of project goals as a progress relative to project planning and the milestones were not evident. On the other hand, the technical accomplishments were evidenced, albeit at a basic level.

Reviewer 3:

The reviewer expressed the need to know how many batteries were tested, how many batches of materials were made, and how varied the surface area and porosity was. The amount of effort put into the project is hard to quantify.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer reported that this project is a collaboration between two divisions of LG Chem that are supported by testing services of national laboratories. Being the case in this project, there is limited scope for the evaluation of the project team's collaboration and coordination with other institutions, and the collaboration with national laboratories was identified as part of the future work.

Reviewer 2:

The reviewer noted that the project does not include many collaborating institutions but, most of the work can be done well in-house.

Reviewer 3:

The reviewer observed that there appears to be no project team collaborations with other institutions, but the validation will be completed in the future.

Question 4: Has the project 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 optimization of the key cell component performance criteria and simplification of the BMS design, are proposed for future work, and if successful, these will certainly contribute to achievement of the goals set by this project and by USABC.

Reviewer 2:

The reviewer noted that the general approaches for future work are broad and appear to cover the main areas for optimization and cost reduction.

Reviewer 3:

The reviewer expressed the need to have access to more specific plans in order to better evaluate future research.

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

Reviewer 1:

The reviewer said that the adoption of Start-Stop technology will have a positive impact, albeit there is a limited impact on petroleum displacement in the automotive sector.

Reviewer 2:

The reviewer stated that the project is directed at the important 12 V Start-Stop Li-ion battery in the 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 reported that the project is adequately resourced at one of the top Li-ion battery company developers and manufacturers.

A Commercially Scalable Process for Silicon Anode Prelithiation: Ionel Stefan (Amprius) - es250

Presenter

Ionel Stefan, Amprius.

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 project motivation is clear, for the method of evaluating Li sources and lithiation techniques is well described and laid out, including performance characteristics and cost. The order of tasks is logical.

Reviewer 2:

The reviewer reported that the project has a single focus on developing a cost effective prelithiation process for the silicon nano-wire anode. Many approaches for prelithiation were evaluated which resulted in several potential candidates.

Reviewer 3:

The reviewer explained that increasing energy-density through pre-lithiation requires a cost-effective method for pre-lithiation of the Si-anode. Whether the pre-lithiation methods investigated in the project are suitable and effective for all Si-morphologies, needs to be demonstrated in order to judge its feasibility and integration with other's efforts. The reviewer added that the design and planning of the project activities and milestones seem appropriate, but one of the barriers identified, shelf-life, is not addressed in the material provided.

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 towards DOE goals.

Reviewer 1:

The reviewer commented that a large amount of work was done on evaluating many possible prelithiation approaches and selecting three of them as the most promising. There appear to be significant technical barriers yet to overcome, so it is not clear that any of these three approaches will show feasibility. The reviewer

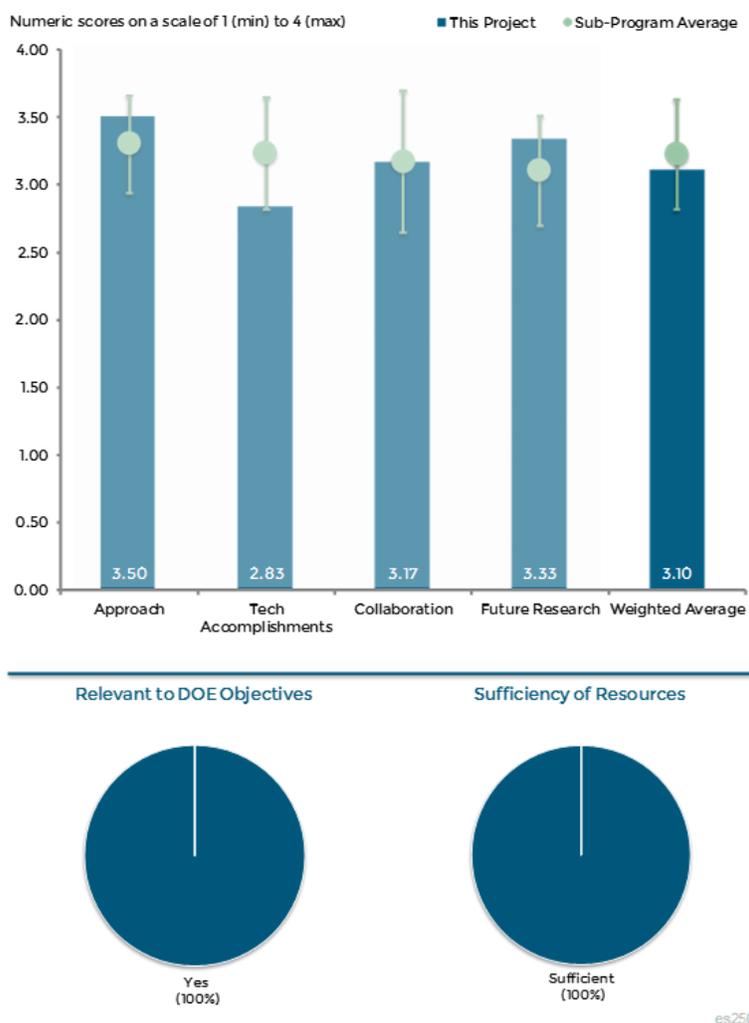


Figure 2-66 A Commercially Scalable Process for Silicon Anode Prelithiation: Ionel Stefan (Amprius) - Electrochemical Energy Storage

expressed that it would be good to continue to look for other strong candidates for prelithiation while working to optimize the three candidates identified in the first part of the project.

Reviewer 2:

The reviewer reported that the concept and potential of pre-lithiation has been demonstrated in this project, although the pre-lithiation techniques evaluated and preselected may depend on the anode morphology. The reviewer expressed the need to know how far the pre-lithiation effects would be applicable to other morphologies. Improvements in capacity retention through pre-lithiation are only effectively demonstrated for pre-lithiation levels greater than 400mAh/g, and it would have been interesting to see some independent testing of performance parameters, for example, reversible capacity and capacity retention.

Reviewer 3:

The reviewer said that words in the graph on Slide 15 provided in PeerNet are hard to read. The reviewer would have liked to see the initial results for cycle lifetime tests, even if only a few cycles.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer commented that while there are no partnerships involved in this testing, it is not thought to be necessary at this time. There are many tasks to be accomplished before it is necessary to involve someone for outside testing.

Reviewer 2:

The reviewer pointed out that the collaboration is not relevant in this project as there is only one partner. This project would definitely benefit from collaboration with other enterprises.

Reviewer 3:

The reviewer observed that this project has a relatively short length of one year and a relatively small budget. This is less oriented to extensive work with other institutions but the project states that it will be relying on vendors for support in doing the project work.

Question 4: Has the project 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 proposed future work is well defined and logical, and thanked the PI for making an easy-to-follow presentation.

Reviewer 2:

The reviewer explained that planning is clear for the remaining months of this short project activity. As a single-participant project, an ex-ante risk-assessment exercise would have been useful to identify and mitigate the external risks needed to achieve the project goals, and in this case, to mitigate risks associated with the timely identification of a supplier of the bespoke pre-lithiation chamber.

Reviewer 3:

The reviewer reported that the project has a short length of only one year, so there may not be sufficient time to identify the cost-effective prelithiation process and demonstrate it on a pilot scale. It would be worthwhile to continue screening for any new prelithiation approaches in parallel in case while working to optimize the selected prelithiation candidates.

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

Reviewer 1:

The reviewer noted that improving the cost of Si electrodes is a great area to explore for increasing energy density for PEV applications.

Reviewer 2:

The reviewer confirmed that the project addresses efforts to improve energy density and cycle life of energy storage systems.

Reviewer 3:

The reviewer explained that the commercial silicon anodes are the leading candidates for next-generation Li-ion batteries for the DOE's objectives. A cost effective prelithiation process is a common barrier for any of the silicon anode designs.

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

Reviewer 1:

The reviewer observed that the project has sufficient resources as long as it follows its intent of engaging vendors where needed and to supplement its internal resources.

Reviewer 2:

The reviewer did not understand how the DOE's funding share is more than the contractor's share if Amprius is the project lead, or why no funds have been transferred during FY 2014.

**12 V SS Battery Development:
Michael Everett (Maxwell) - es251**

Presenter

Michael Everett, Maxwell.

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 reported that the project approach is planned and scheduled well. In this project, critical barriers to developing a lead-free, more durable, and lighter 12 V alternative technology in a hybrid format are cost and complexity. The feasibility of the system being developed overcoming these barriers is questionable, particularly with respect to the energy management system and gas management. Integration of an ultra-capacitor for power in a 12 V system delivery is novel, especially at low-temperature.

Reviewer 2:

The reviewer commented that the approach is well-defined but requires performance based on the identification of additives that will lead to performance requirements based on their reactivity. The reviewer asked if there is a backup plan if such additives are not identified that both solve these problems and are cost effective.

Reviewer 3:

The reviewer stated that the project has a broad approach with a focus on overcoming the gas formation and mitigation barrier as a key enabling step.

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 towards DOE goals.

Reviewer 1:

The reviewer explained that the evaluation of a suitable electrolyte is an important aspect of this project together with management of gas, and that few results are presented to evidence the technical accomplishments claimed, e.g., results supporting the selection of electrolytes and results demonstrating the effectiveness of the gas suppression additive. The interchangeable use of the terms pouch, prismatic, and pouch prismatic to describe ultracapacitor cell format is both confusing and inconsistent.

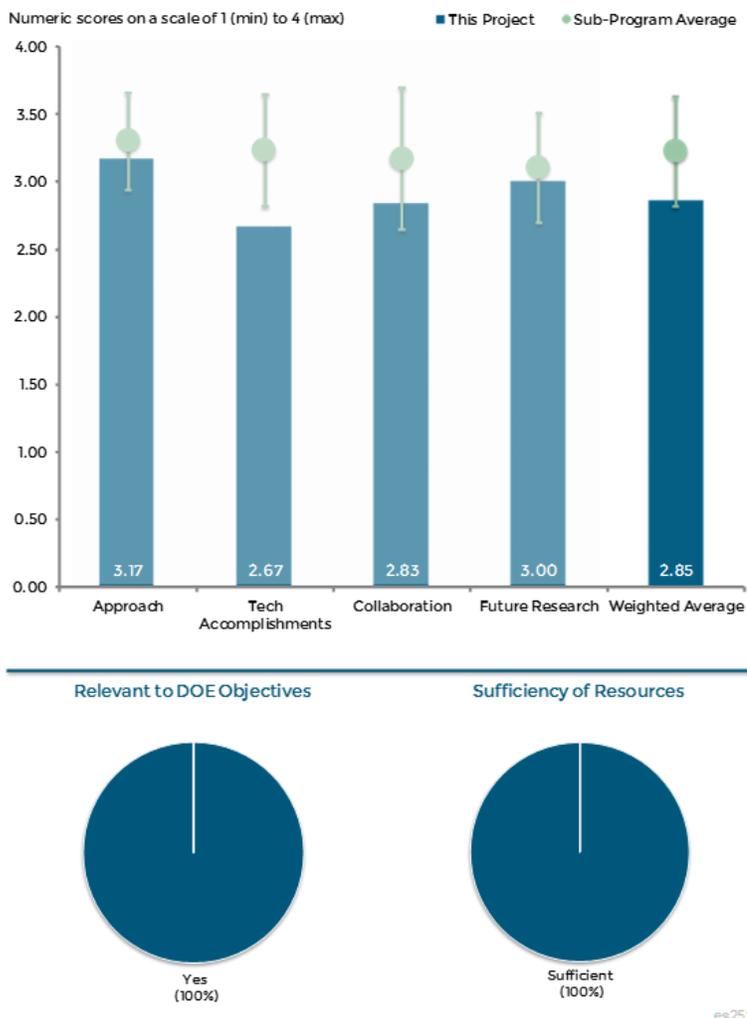


Figure 2-68 12 V SS Battery Development: Michael Everett (Maxwell) - Electrochemical Energy Storage

Reviewer 2:

The reviewer reported that a considerable amount of work was done on evaluating electrolytes with acceptable gas formation with two candidates identified for further work. It would be advisable to continue screening for better electrolytes and to evaluate separators and other components that might lower the gas formation at high temperatures. The reviewer added that depending on a gas getter of some type to mitigate, the gas level may not be an approach that provides consistent quality.

Reviewer 3:

The reviewer explained that it was stated that two promising acetonitrile-based electrolyte formulations were identified. The reviewer asked what made them better than the others and what components were unique, what electrolytes are being tested in this project that are different from what others have evaluated, or if the same, what the motivation is for retesting them. The electrolyte screening work would be of interest to others in the field. The reviewer also expressed an interest to understand if there any plans to disseminate knowledge through peer-reviewed literature.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer noted that project team's collaboration with two national laboratories is an integral part of the project.

Reviewer 2:

The reviewer observed that ANL and NREL are listed as collaborators but it is not clear if and in how far the collaboration is realized.

Reviewer 3:

The reviewer said that it is unclear what work was done by Maxwell verses the USABC within the proposal, and understands that NREL does thermal modeling. The reviewer expressed the need to know what kind of thermal testing has and will NREL do that is specific to this battery system, and if the work is ongoing or to be in the future.

Question 4: Has the project 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 degree to which the cost and energy management system barriers are overcome are addressed in the future work of this project. Demonstration of the proof of concept system is an important future milestone and independent testing by the national laboratories will provide important proof.

Reviewer 2:

The reviewer stated that the ultracapacitor component of the project needs significant design improvements, especially for acceptable gas formation levels. Broader efforts are needed to get this design ready on schedule for building into the battery system and evaluating it for performance against the project targets.

Reviewer 3:

The reviewer explained that specifics for future work are not enough to evaluate its merit. For example, in one case, 20-plus carbonate-based formulations have been tested with no promising candidates. The reviewer asked what will be done in the next round of testing that is different from what has already been tested that will increase the likelihood of success.

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

Reviewer 1:

The reviewer stated that Start-Stop technology offers some fuel economy gains which, to some degree, contributes to objectives towards petroleum displacement.

Reviewer 2:

The reviewer noted that the 12V Start-Stop lithium-ion battery and ultracapacitor combination is part of the DOE's objectives for vehicles.

Reviewer 3:

The reviewer said that the improvements in energy storage systems could allow for decreased utilization of coal burning power plants or of renewable energy sources.

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 being done at the leading ultracapacitor company in the United States with support by two national laboratories for the testing.

Reviewer 2:

The reviewer remarked that without access to the budget or description of facilities, it is not clear if the resources available are appropriate or not.

New High-Energy Electrochemical Couple for Automotive Application: Xiao-Qing Yang (Brookhaven National Laboratory) - es255

Presenter

Xiao-Qing Yang, Brookhaven National Laboratory.

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:

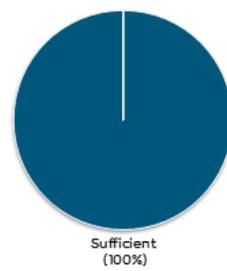
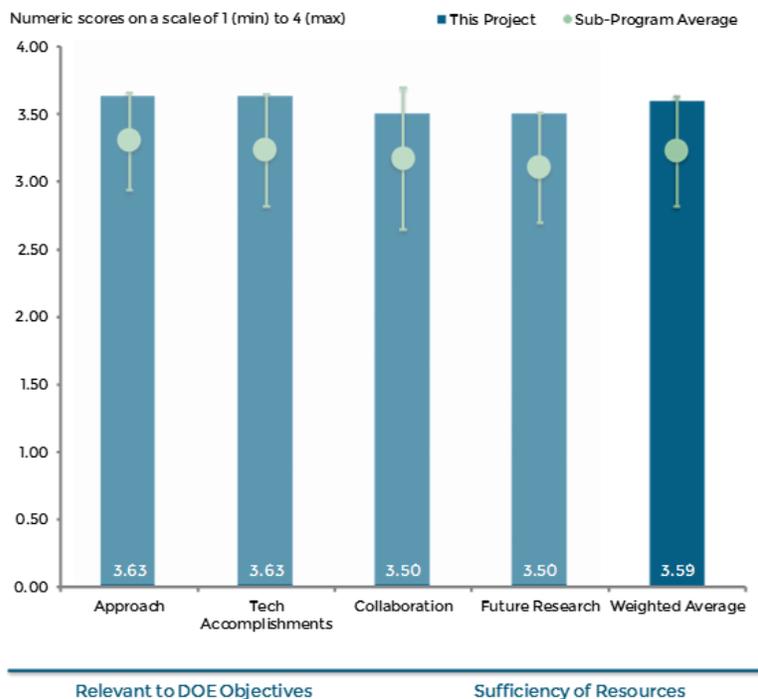
The reviewer stated that the in-situ time-resolved X-ray diffraction (TR-XRD) coupled with mass spectroscopy (MS) was interesting and the data collected was very compelling. It shows that the disordered spinel and final rock-salt structure are formed as the charged cathode powder is subject to higher temperatures, and that the stability-gain reported for the gradient material is very clear.

Reviewer 2:

The reviewer expressed that the principals laid out in a very well organized approach to developing techniques that would allow a more fundamental understanding of key active material characterization. The goals were clear and the follow through stayed on task.

Reviewer 3:

The reviewer explained that the work aims to analyze and compare concentration gradient (CG) NMC622 and NMC622 without CG bulk, and that the thermal stability of this material is a critical point as it is one of the major drawbacks of the material, so the work is of major importance. TR-XRD and soft X-ray absorption spectroscopy (SXAS) are used as methods, and additionally, transmission X-ray microscopy (TXM) is utilized to visualize the elemental distribution of Ni, Mn and cobalt (Co) within the CG NMC622. The reviewer added that this work is thoroughly performed with emphasis on detail and gives significant input on the thermal stability of NMC622 materials.



es255

Figure 2-69 New High-Energy Electrochemical Couple for Automotive Application: Xiao-Qing Yang (Brookhaven National Laboratory) - Electrochemical Energy Storage

Reviewer 4:

The reviewer stated that TR-XRD may provide less detailed structural information compared to the conventional approach. For SXAS, the ability to decipher both the surface and bulk structure is very useful and powerful.

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 towards DOE goals.

Reviewer 1:

The reviewer stated that the demonstration of an increased thermal stability for the gradient cathode powder was a good accomplishment. The TR-XRD/MS plots and the contour plot were very easy to follow, and the effect of temperature was clearly displayed.

Reviewer 2:

The reviewer reported that the progress of the first year is impressive and depicts also the good collaboration in this project, and the chosen techniques and the approach are well suited for the tasks and ensure the progress. Detailed and elaborated results are shown correlating the thermal stability of bulk NMC622 and CG NMC622 to the phase-transformation of the material. The reviewer also said that the results are important and can provide significant information towards the improvement of these materials, but more work is needed in order to correlate the material properties to electro-chemical performance and the lifetime. It is appreciated that this is already addressed in the proposed future research.

Reviewer 3:

The reviewer noted that the project team has good progress on both the thermal stability studies and the metal mapping work.

Reviewer 4:

The reviewer noted that the project team well demonstrated its applicability and unique capability with CG materials, but it is not very clear about the need of TXM.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer observed that the project team has clearly shown that it has good interaction with other institutions.

Reviewer 2:

The reviewer said that the project team's collaboration combines several institutes and groups, and is well coordinated based on the strengths and capabilities of each partner.

Reviewer 3:

The reviewer noted that the project team's collaboration is well described.

Reviewer 4:

The reviewer stated that project team's collaborations appeared to be with very high quality partners, but a slightly more detailed description of who was doing what would be appreciated.

Question 4: Has the project 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 work is well coordinated and balanced. The reviewer commented the mentioned expansion of the collaboration should be described in some more detail for which partners and/or which tasks. It is recommended to focus on the correlation of the material properties to electrochemical performance and derive design guidelines for future concentration gradient materials.

Reviewer 2:

The reviewer noted that the project team's collaboration with U.S. academic research institutions will be important for quick dissemination of the advanced technologies.

Reviewer 3:

The reviewer believed that the tools have shown good usefulness in the areas of interest, and hoped these tools can be used on other active material systems in the future.

Reviewer 4:

The reviewer commented that as mentioned by the authors, the thermal abuse tolerance will be extended using their in situ method, and that the addition of surface and bulk sensitivity analysis will be very useful. The project team may end up providing some light into the mechanism of degradation and potential mitigation strategies.

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

Reviewer 1:

The reviewer remarked that yes, the project is very relevant to the objective of petroleum displacement.

Reviewer 2:

The reviewer stated that the diagnostics study for safety and calendar and cycle life is essential to improve battery performance, which is significant for the achievement of DOE's objectives.

Reviewer 3:

The reviewer said that important information is provided on the thermal stability of NMC622 materials, with and without CG.

Reviewer 4:

The reviewer expressed that it is welcoming to see some solid fundamental material analysis aimed at key attributes affecting material behavior.

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 project's resources are adequate and well allocated to achieve the goals of the project.

Reviewer 2:

The reviewer observed that the project's resources seems sufficient, however, if the authors tried to extended their study into many more cathode powders, the resources may not be sufficient.

Reviewer 3:

The reviewer commented that a detailed budget is not provided.

3M IC3P - Research Focus: Jagat Singh (3M) - es256

Presenter

Kevin Eberman, 3M.

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 explained that the investigation phase of the research provides a well-executed study of the target performance parameter and ultimately provides some real insight into potential causes of issues within the Si anode system.

Reviewer 2:

The reviewer stated that the author seems much focused on the Si alloy challenges, and FEC is playing an important positive role. However, gassing seems to be one the main problems to focus on, and the authors are working on it.

Reviewer 3:

The reviewer said that the PI is not very clear about the strategy to solve the problems. The impact of additive materials on cathode side must be considered, for it is well known that FEC has impact on cathode.

Reviewer 4:

The reviewer commented that no explanation of the scientific approach is given in the presentation, and obviously it is focusing on the failure mechanisms during cycling of the Si-alloy. Effects of electrolyte mixture, cathode material and, for one example, the associated volume exchange are being investigated. The reviewer added that this work seems more like engineering work of test and see what happens, than scientific work to find causes scientifically and solve the problems, and is in particular disappointing as the project es255 was understood as deep dive linked to project es210.

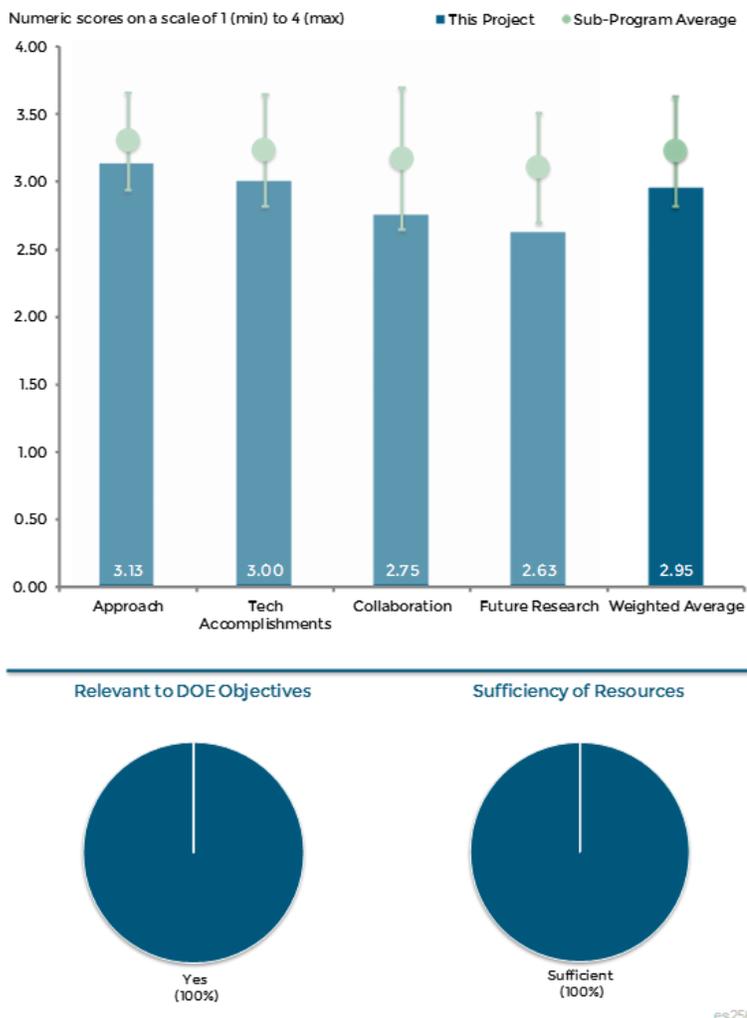


Figure 2-70 3M IC3P - Research Focus: Jagat Singh (3M) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer reported that the authors made real progress on the sudden fade mechanism due to the silicon anode, but at some point, the authors should mention what is meant by the term improve microstructure. Electrolyte with VC-ethylene acrylic (EA) solvent seems to greatly help. Similarly, the NMC cathode seems to be playing a role in mitigating the sudden fade. The reviewer commented that at some point, the authors should provide some information about the mechanism behind that positive effect.

Reviewer 2:

The reviewer explained that the progress in addressing performance issues provides some interesting avenues for exploration, and the development for these approaches is less compelling than the initial evaluation, with some of the outcomes ranging from interesting to perplexing. The observation of FEC gassing seems to be developing as a common issue in the Si anode field and needs to be driven to ground. The reviewer added that the observation of performance differences based on cathode choice alone, are very perplexing, and while it is appreciated that they are included, it is somewhat perplexing on the potential mechanism.

Reviewer 3:

The reviewer observed that some changes, for example, electrolyte or matching cathode, showed the improvement of lifetime. Such results can be important for further development of Si-based materials to achieve longer cycle life. However, the reviewer commented that explanations are missing why such changes resulted in the improvement. In order to make further simple and logical investigations, the effect of such electrolyte or cathode change on the Si-alloy needs to be better understood. The reviewer added that in particular, the improvements shown are small and the present results are far away from the targets for automotive applications.

Reviewer 4:

The reviewer commented that all the project team's results look ad-hoc based on test.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that 3M Company is collaborating strongly with other institutions such as General Motors Company, LBNL, ARL, and Umicore.

Reviewer 2:

The reviewer remarked that there is no collaboration listed, but without details, the reviewer would not consider this to be a negative. As mentioned, the work appears to be high quality.

Reviewer 3:

The reviewer noted that from the presentation, there was no cooperation apparent.

Reviewer 4:

The reviewer commented that there was no clear description for collaboration.

Question 4: Has the project 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 in the area of future work, the project team has done a good job. Further studies related to the effect observed on the sudden fade by the different cathode powders should be pursued.

Reviewer 2:

The reviewer remarked that future work is not referenced in the enclosed document. It is perhaps somewhere else where this reviewer does not have access.

Reviewer 3:

The reviewer noted that proposed future work was not described.

Reviewer 4:

The reviewer commented no future plan.

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

Reviewer 1:

The reviewer remarked that yes, understanding and improvement of life time of Si based material is important to achieve the DOE's objectives, as Si based material have higher capacity than current typical graphite which can lead to the realization of the higher energy density Li-ion battery cells.

Reviewer 2:

The reviewer said that yes, the project is very relevant to the objective of petroleum displacement. The development of high-energy Si alloy anodes will result in higher energy batteries.

Reviewer 3:

The reviewer stated that this work provides at least some insight into mechanistic issues associated with Si anode performance. Much more work is needed, but progress will be very sporadic without more work like this being developed.

Reviewer 4:

The reviewer noted that Si alloy is one of the important materials for achieving the DOE's objectives, but the cause of sudden fade must be resolved.

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 project's resources seems to be sufficient.

Reviewer 2:

The reviewer stated that project's resources were not given in the presentation.

Reviewer 3:

The reviewer noted that project team provided no detailed budget information.

Ion-Exchanged Derived Cathodes (IE-LL_NCM) for High-Energy Density Lithium-Ion Batteries: Christopher Johnson (Argonne National Laboratory) - es257

Presenter

Christopher Johnson, Argonne National Laboratory.

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 it is a very interesting approach that tries to stabilize the LMR-NMC cathode through new synthetic routes. The stacking faults approach of ion exchanged-layered layered-nickel cobalt manganese (IE-LL-NCM) followed by the authors seems to be a reasonable good alternative and the team has done a lot of work in that area; the reviewer remarked very focused.

Reviewer 2:

The reviewer said that according to the concept of project es213, this work shows two deep dives by ANL and LBNL into the two approaches to improve the capacity of the cathode material IE-HE-NMC and or modified NMC to allow for higher voltages. The scientific approach is well chosen and the techniques well suited to reveal substantial understanding of fundamental processes.

Reviewer 3:

The reviewer commented that the interest in attempting a new synthesis process as a method to modify the behavior of the Li-Rich active material system, is a worthy goal. It is not completely clear that the structural areas that can conceivably be modified by the proposed process line-up with a potential performance improvement, but making the attempt is probably reasonable.

Reviewer 4:

The reviewer stated that rate-capability also must be considered. Surface coating alone cannot solve the high-power properties.

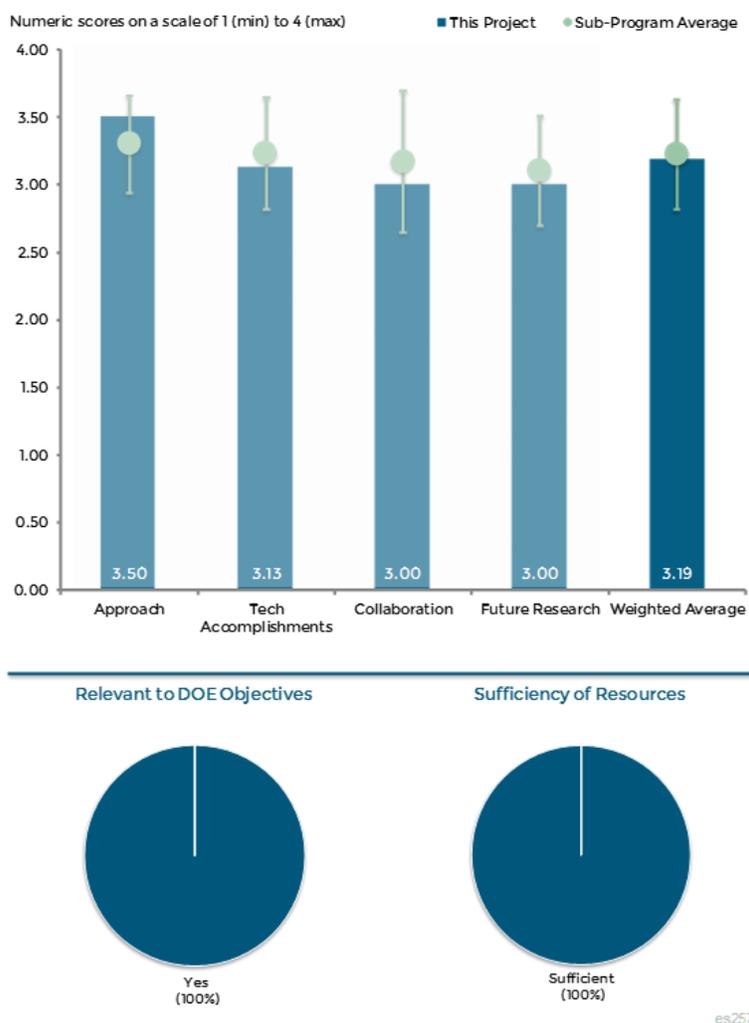


Figure 2-71 Ion-Exchanged Derived Cathodes (IE-LL_NCM) for High-Energy Density Lithium-Ion Batteries: Christopher Johnson (Argonne National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer explained that the project team has made significant progress, and in particular, the results of LBNL are impressive. For the IE-HE-NMC, the progress in the synthesis of the material is also very good. But the reviewer recommended that the team think about additional analytical techniques beyond XRD, to further strengthen the understanding of the synthesis parameters, and to link it to the material characteristics and finally electrochemical and lifetime results.

Reviewer 2:

The reviewer explained that it will be interesting to know how much cathode material the authors can produce in one batch, for the researchers already mentioned that the scale-up is in the horizon. At some point, it will be of great interest to know the reproducibility of the ion exchange process in more detail. The reviewer added that the authors mentioned that there is some composition variance in the process.

Reviewer 3:

The reviewer noted that the demonstrated cycle-number is too small to be competitive to other materials.

Reviewer 4:

The reviewer stated that the signals from the material produced by the process do not indicate a high-probability of success in addressing the target performance characteristics.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team's collaboration seems to be very good with Farasis Energy, which is a battery company, and that is very good.

Reviewer 2:

The reviewer said that the research seems to be well connected with the other project partners. Testing this material in commercial grade cells from Farasis Energy might unveil its full potential.

Reviewer 3:

The reviewer commented that there is very little project team collaboration at this stage, which is perhaps reasonable.

Reviewer 4:

The reviewer noted that the project team's collaboration is not clear.

Question 4: Has the project 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 it seems that further exploration on the synthetic routes is a good alternative. Further characterization of the powders should be done, and additional insight into how scalable are these processes, should be considered too.

Reviewer 2:

The reviewer explained that the proposed future research is justified and continues to follow the route already taken. Input by the project partners can further elaborate the work and it will be interesting how the lower-voltage fade influences the material performance in larger cell formats.

Reviewer 3:

The reviewer commented that it is not clear that the current results suggest a strong case for further experimentation. As a further note, it would be important to know that if the process were capable of producing the intended structural and therefore performance characteristics. The reviewer asked does it have feasibility as a commercial process.

Reviewer 4:

The reviewer noted that the project team has no future work focused on rate-capability.

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

Reviewer 1:

The reviewer said that yes, the project work is very relevant to the objective of petroleum displacement. How to mitigate the voltage-fade issue for the LMR-NMC layered compounds is a step in the right direction.

Reviewer 2:

The reviewer stated that high-capacity cathode material is an important component to DOE's development path.

Reviewer 3:

The reviewer commented that the project work is directly directed towards achieving battery energy density targets for xEVs.

Reviewer 4:

The reviewer noted that that the new cathode materials are necessary to improve the energy density of Li-ion cells.

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 that the project is almost complete at this time and that the resources were good.

Reviewer 2:

The reviewer said that the project's dedicated resources are sufficient.

Reviewer 3:

The reviewer noted that the project team provided no detailed information about budget.

**Envia IC3P - Research Focus:
Robert Kostecki (Lawrence
Berkeley National Laboratory) -
es258**

Presenter

Robert Kostecki, Lawrence Berkeley National Laboratory.

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 research is well focused, and that the analytical information obtained with in-situ Raman seems very valuable and is giving important information at the surface and electrolyte interphase. The data collected with the HCMR baseline materials gave very useful hints to Envia Systems.

Reviewer 2:

The reviewer expressed that there is an appreciation for the effort to investigate mechanistic causes for materials performance. Applying multiple analytical techniques and attempting to reconcile their collective results is also appreciated.

Reviewer 3:

The reviewer explained that the project is well-designed to investigate the fundamental problem of the direct current resistance (DCR) rise in HCMR cathodes. The multi-scale approach and the combination of spectroscopic techniques, calculations, and electrochemical investigations is well thought through and may provide new insight into the structural problems of the material.

Reviewer 4:

The reviewer stated that the approach is not very clear about doping study for the goal of the project is to understand DCR increase.

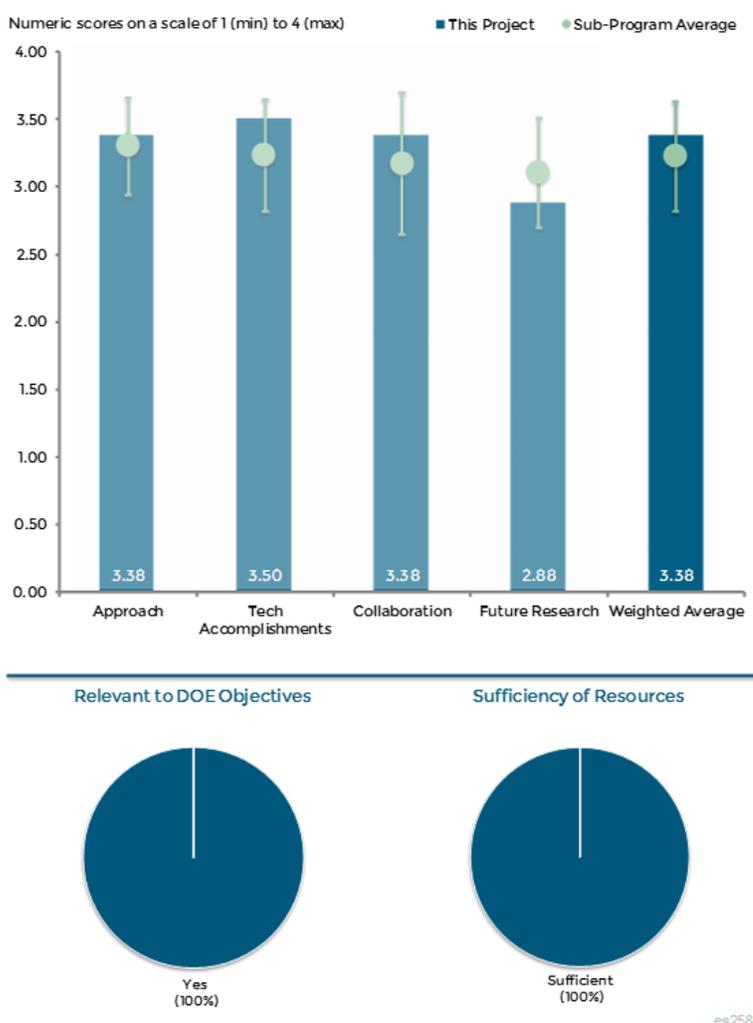


Figure 2-72 Envia IC3P - Research Focus: Robert Kostecki (Lawrence Berkeley National Laboratory) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer commented that overall, the project team has shown great progress. The in-situ Raman data was nicely utilized to confirm the formation of spinel-like structure after cycling.

Reviewer 2:

The reviewer stated that the development of a preliminary model for resistance increase is a positive step in the understanding of performance related to the HCMR material.

Reviewer 3:

The reviewer explained that the outcome of the project is good and the combination of the different techniques is very useful. Considering the dynamic changes on the surface of the electrode, it might be very interesting to also investigate the electrolyte at different potentials and see if the FTIR observed changes correspond to chemical changes in the electrolyte at these potentials. The reviewer added that the calculations showing the effect of doping on the Mn migration are interesting and opens new possibilities for material design.

Reviewer 4:

The reviewer commented that it is not clear about the explanation on higher DCR change at cycle 5 than cycle 100, for correlation between DCR and Li⁺ diffusivity is not strong against the claim in the summary. There are significant DCR changes within a single discharge as well as prolonged cycles, however, there is no change of Li⁺ diffusivity with prolonged cycling.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team's collaboration between the different institutions has been very strong. General Motors, ORNL, and Envia Systems were involved and showed good coordination.

Reviewer 2:

The reviewer noted that a strong, diversified team seems to have produced good integrated results.

Reviewer 3:

The reviewer remarked that the project team's collaboration between the different groups involved is obvious, and that the work is well coordinated.

Reviewer 4:

The reviewer noted that the project has no detailed description or activity about collaboration.

Question 4: Has the project 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 authors have done very comprehensive analytical work. After down-selecting the best composition, the team will be able to use the very promising diagnostic method described in the work, to move the project forward.

Reviewer 2:

The reviewer stated that the future research is not outlined in the presentation, and expressed an apology if there is a separate section which was missed.

Reviewer 3:

The reviewer reported that the presentation did not contain information on proposed future research, and that in the ranking, it was assumed that the groups continue the present approach. It is recommended to further link the results of the different techniques, and to even enhance the identification of the fundamental mechanisms.

Reviewer 4:

The reviewer commented that no specific future plan is given.

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

Reviewer 1:

The reviewer stated that the specific outcome of mechanistic understanding of this material is important for future research direction, as is the technique development can be applied to other materials.

Reviewer 2:

The reviewer said that yes, the project is very much aligned with petroleum replacement. The use of high-capacity cathode powder is badly needed in this area.

Reviewer 3:

The reviewer remarked that yes, the topic addresses one of the main risk items for layered-layered materials which is the low-power capability, and therefore, low-usable energy.

Reviewer 4:

The reviewer commented that understanding the DCR rise in high-energy density materials is essential for developing high-energy density 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 observed that the project's resources seems to be adequate. The project is finishing this year and the amount of data produced indicates that the resources have been well utilized.

Reviewer 2:

The reviewer noted that the project's resources were not given.

Reviewer 3:

The reviewer commented that no detailed information about budget is provided.

Prospects and Challenges of Nickel-Rich Layered Oxide Cathodes: Arumugam Manthiram (University of Texas at Austin) - es259

Presenter

Arumugam Manthiram, University of Texas at Austin.

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 reported that the project work is focusing on synthesizing Ni-rich layered cathodes with a target of 220 mAh/g capacity, and is one of the most promising candidates to reach the DOE capacity targets. This approach of the work is very good starting with the synthesis and accordingly, process parameters. The reviewer added that the work thoroughly analyses the subsequent influence on particle size, morphology, properties, and electro-chemical performance, which is also very good.

Reviewer 2:

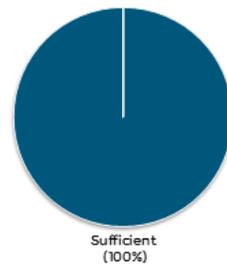
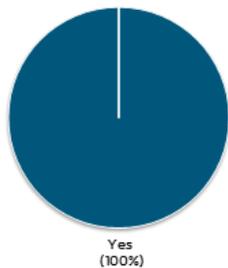
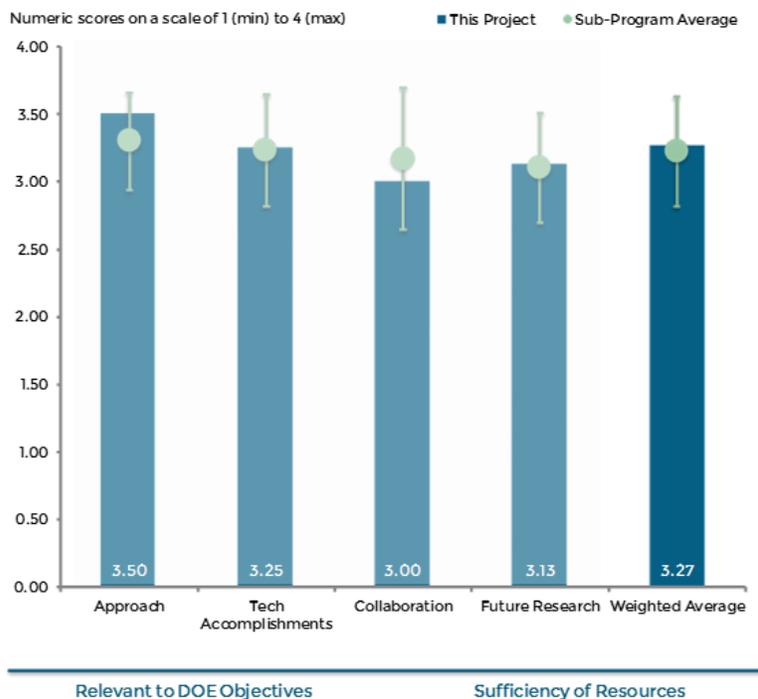
The reviewer said that the approach is good for it includes a comprehensive analysis of various parameters which affect the performance of the nickel-rich materials.

Reviewer 3:

The reviewer stated that the approach is effective in overcoming most barriers, for Ni-rich and gradient cathode powders are not easy to produce. At some point, a scale-up discussion should be introduced.

Reviewer 4:

The reviewer commented that this material is not gradient material and it may still have a problem related to mismatch between components.



es259

Figure 2-73 Prospects and Challenges of Nickel-Rich Layered Oxide Cathodes: Arumugam Manthiram (University of Texas at Austin) - Electrochemical Energy Storage

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 towards DOE goals.

Reviewer 1:

The reviewer stated that the data and techniques associated with the characterization effort seem to be useful analytical techniques and results.

Reviewer 2:

The reviewer reported that substantial progress was shown for number of variants were synthesized and evaluated, and the fundamental understanding of the investigated sensitivities was increased. Even though improvements have been shown, it is still open how the targets can be reached. Moreover, the influence of the electrolyte on the performance of the cell was not discussed. The reviewer recommended that the team analyze the present results with the focus on a strategy to derive a design directive for the next material generation that can meet the target.

Reviewer 3:

The reviewer explained that it is clear that the constant concentration gradient is produced using a continuously stirred tank reactor, but it is not very clear how the authors can produce the concentration gradient powder. It seems that in that case, the project team will have to use a batch process.

Reviewer 4:

The reviewer commented that the project team needs to explain the observed phenomena in order to improve the performance. The relation between the particle size and impedance change is not clear and the demonstrated cycling life is not impressive.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that it seems that the author is coordinating discussion with other groups.

Reviewer 2:

The reviewer observed that most of the collaborations seem to involve monthly project discussion, but is not quite sure what this means or what it accomplishes.

Reviewer 3:

The reviewer noted that the project team's collaboration is well established.

Reviewer 4:

The reviewer remarked that the project work is done within a strong collaboration of partners. It would have been helpful to show in this presentation the interfaces to the partners, in particular, those who influence this work, for example, the influence of electrolytes as provided by ANL.

Question 4: Has the project 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 remaining project challenges are clearly recognized and the future work addresses these challenges. As the remaining time is quite short, it might be necessary to focus on the most promising action items.

Reviewer 2:

The reviewer said that the project's future work is effective; however, more examples of gradient powders are needed. Reproducibility of the results should be mentioned.

Reviewer 3:

The reviewer stated that the project team's goals are reasonable, of course, and well known. However, whether the effort can actually enable improvement toward these goals is yet to be determined.

Reviewer 4:

The reviewer commented that the project team needs to first understand the stabilization mechanism of the target materials. Then, the team needs to evaluate the long-term cycle performance.

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

Reviewer 1:

The reviewer stated that developing a fundamental understanding of the factor that control the battery performance of high-energy density materials is urgently needed to achieve the DOE objectives.

Reviewer 2:

The reviewer explained that the project is very relevant to the DOE objectives, as a cathode with increased capacity is necessary in order to achieve the targets for future automotive applications.

Reviewer 3:

The reviewer said that yes, the project work is very relevant for the production of high-energy batteries.

Reviewer 4:

The reviewer stated that the high-energy cathode materials are an important component of advanced cell concepts.

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's resources are sufficient for the amount of powder and different powders produced.

Reviewer 2:

The reviewer stated the resource amount and allocation are sufficient in order to achieve the targets of the project.

Reviewer 3:

The reviewer noted that detailed information about budget is not provided.

Materials Development for High-energy High Power Battery Exceeding PHEV-40 Requirements: Jane Rempel (TIAX) - es260

Presenter

Jane Rempel, TIAX.

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:

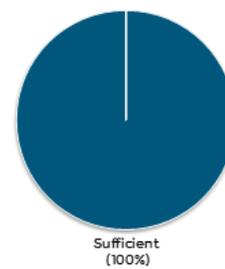
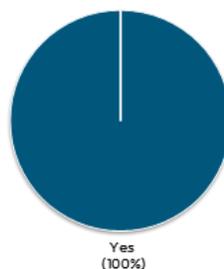
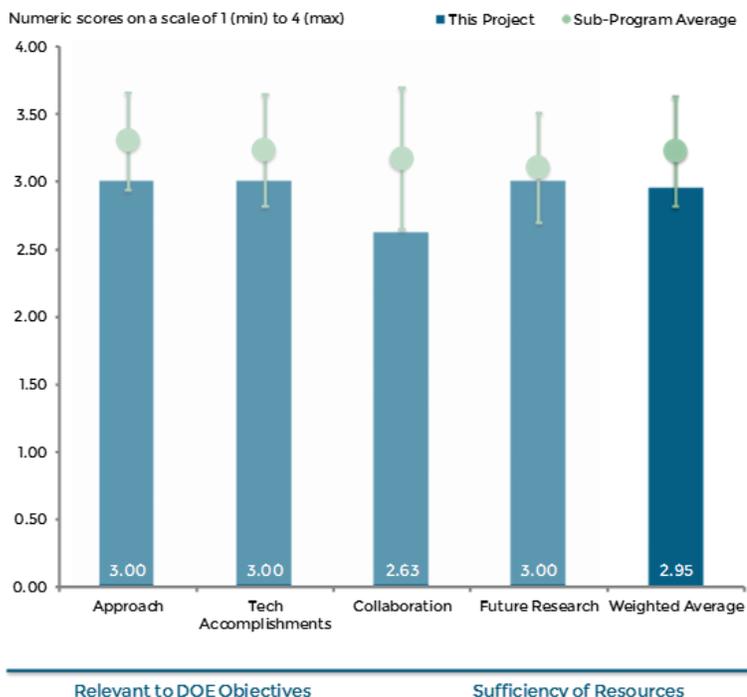
The reviewer believed it is very difficult to solve the technical issues when a supplier is working with the powder in another company. However, the authors have done a good job in this area and have shown very interesting progress in terms of cathode and anode capacity.

Reviewer 2:

The reviewer reported that as with many of the programs that include the optimization of a high-capacity cathode and Si based anode, the cathode work in this project is much further along. The CAM-7 material appears to have been given a modest performance improvement through material optimization. The reviewer went on to say that the Si anode portion of the program is less clear, for at the moment, it appears to be a screening program aimed at developing the empirical relationships between various material and electrochemical options. The reviewer stated that it was thought that it is difficult to assess the program in its own right, as the program appears to be taking proprietary anode materials from various sources and simply characterizing them for behavior. The quality of the work appears to be quite acceptable, and so, is not an issue.

Reviewer 3:

The reviewer explained that the principal approach of using Ni-rich cathode material and Si based anode material is reasonable, but taking into account that the contractor is following this development path for the cathode material since many years, a clear strategy or approach is not obvious on how to improve the material to meet the targets. On the anode side, there is no explanation how to finally decide on the material or to further develop the materials.



es260

Figure 2-74 Materials Development for High-energy High Power Battery Exceeding PHEV-40 Requirements: Jane Rempel (TIAX) - Electrochemical Energy Storage

Reviewer 4:

The reviewer stated that the approaches main strategy is doping for cathode and Nano-sized composite for the anode. Even though they are typical approaches, it is not clear they are unique approaches for solving the related problems. Also, the reviewer added that the project team is mainly relying on the vendors' materials. An optimization process may be needed rather than trying via trial and error.

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 towards DOE goals.

Reviewer 1:

The reviewer reported that that the project team's progress has been good, for the authors showed good data, but at some point, the authors should provide additional information related to the powders they are using. If not, or because of proprietary information that cannot be disclosed, the authors should provide some information on how reproducible the data is that they can obtain from the different suppliers, and how reliable are those products.

Reviewer 2:

The reviewer explained that as per the approach discussion, a modest improvement of the CAM-7 material was demonstrated and is a solid accomplishment. It is less clear that contributions to the anode field have been produced. The reviewer perceived that everyone is testing everyone else's proprietary materials, and that they are all coming up with the same empirical conclusions, but with little fundamental progress in the field. The reviewer stated that this work is a quite a solid version of that progress, and that this comment is not negative for this particular discussion. This is more of a comment in terms of a high-level view of the variety of work that is occurring.

Reviewer 3:

The reviewer commented that some conclusions are quite general, such as that the lower capacity materials exhibit longer cycle life without loss of Si contact, and that capacity retention and Coulombic efficiency decrease at higher Si levels. The lower voltage cutoff can also be increased in full cells to improve cycle life, however, it leads to reduction in cathode utilization. The reviewer also stated that the project team may need to plan some strategy rather than trying combination of materials from different vendors.

Reviewer 4:

The reviewer reported that some progress was made with the lithium nickel oxide (LNO) material, however the results are still far behind the target. Moreover, most half-cell investigations stop at 4.2 V, which will lead to cell cut-off voltage even below 4.2 V, and this will not fulfill the capacity targets and the cycling results might not be very meaningful. It is also recommended to include a side-by-side comparison of the TIAX LLC material with a standard nickel-rich NMC. The reviewer also stated that in the SI-based anode development, no clear strategy can be seen to meet the targets for the results show minor improvements on cycle life but do on the expense of capacity. No detailed analysis of the degradation mechanisms and possible modifications towards substantial improvements were given. The reviewer went on to say that milestone overview only states as scheduled, and it is unclear which milestones are completed and which have been missed, and also see es209.

Question 3: Collaboration and coordination with other institutions.

Reviewer 1:

The reviewer stated that the project team's collaboration with other groups does not seem to be a strong point, and the authors already explained the reasons. There is hope that in the future that involved researchers will be able to get additional insights.

Reviewer 2:

The reviewer explained that the project is lacking support from academic institutions and research centers, and the know-how input by the suppliers cannot be judged with the present data. It would be a probable advantage to establish a collaboration with one of the Si-material suppliers and/or cell manufacturers in order to ensure the progress in this field and to make the program successful.

Reviewer 3:

The reviewer stated that the project team's main collaborators are material suppliers, and it can be expected that there will be some limitations in the exchanging of data and outcomes, which also hinders closer collaborations.

Question 4: Has the project 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 approach mentioned by the authors seems appropriate, for the team will finalize cathode composition, continue with optimizations, and continue with tests based on 18650 cells. In the future, the authors should say something about electrode fabrication. The reviewer expressed a need to understand how difficult it is to scale up a pasting process with these new Si-containing anodes, for example. The reviewer asked how difficult is the pre-lithiation process, is it scalable, and how labor intensive.

Reviewer 2:

The reviewer commented that the proposed future work is repeating the milestone but does not state which specific research activity is started to improve the materials and finally cell performance. With only a few months left in the program, it is unlikely that the project will reach all milestones and targets.

Reviewer 3:

The reviewer stated that the power capability must be considered, for the demonstrated cycling performance is still not impressive.

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

Reviewer 1:

The reviewer said that yes, the project very much supports the overall DOE objective of petroleum displacement. The study on high-energy cathodes and anodes are definitely in the right direction.

Reviewer 2:

The reviewer commented that the high-capacity cells are a critical component to the DOE's development path.

Reviewer 3:

The reviewer remarked that yes, the development of a high-capacity cathode material would enable higher energy density batteries and automotive packs.

Reviewer 4:

The reviewer noted that the high-energy-density and power-density battery systems are necessary for the achievement of the 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 commented that it is hard to know if the resources are insufficient without knowing additional details about the working relationships the authors have with the different suppliers.

Reviewer 2:

The reviewer noted that no detailed information about budget is provided.

Acronyms and Abbreviations

| | |
|------------------|--|
| 3D | Three Dimensional |
| ABR | Advanced Battery Research |
| AC | Alternating current |
| ADP | Advanced drying process |
| Ah | Ampere-hour |
| ALD | Atomic Layer Deposition |
| AlF ₃ | Aluminum fluoride |
| AMR | Annual Merit Review |
| ANL | Argonne National Laboratory |
| ARK | Abuse Reaction Kinetics |
| ARL | Army Research Lab |
| ARPA-E | Advanced Research Projects Agency - Energy |
| ATR | Attenuated Total Reflectance |
| BATT | Batteries for Advanced Transportation Technologies |
| BES | Office of Basic Energy Sciences |
| BMR | Battery Materials Research |
| BMS | Battery Management System |
| BNL | Brookhaven National Laboratory |
| C | Carbon |
| CAD | Computer-aided design |
| CAE | Computer-aided engineering |
| CAEBAT | Computer-aided engineering of batteries |
| CAFE | Corporate Average Fuel Economy |
| CAMP | Cell Analysis, Modeling, and Prototyping |
| CEI | Cathode electrolyte interphase |
| CG | Concentration gradient |
| CMC | Carboxymethyl Cellulose |

| | |
|-------|--|
| CNT | Carbon Nanotubes |
| Co | Cobalt |
| Cr | Chromium |
| CSTR | Continually stirred tank reactor |
| Cu | Copper |
| DC | Direct current |
| DCR | Direct current resistance |
| DFT | Density Functional Theory |
| DoD | Depth of discharge |
| DOE | Department of Energy |
| DPP | Dynamic particle-packing |
| DSC | Differential Scanning Calorimetry |
| EA | Ethylene acrylic |
| EC | Ethylene Carbonate |
| ECT | Electrochemical-Thermal Coupling |
| EDM | Electrode domain model |
| EDS | Energy Dispersive X-ray Spectroscopy |
| EELS | Electron Energy Loss Spectroscopy |
| EIS | Electrochemical Impedance Spectroscopy |
| EOL | End-of-life |
| EPA | U.S. Environmental Protection Agency |
| EPR | Electron Paramagnetic Resonance |
| EV | Electric Vehicle |
| EXAFS | Extended X-ray Absorption Fine Structure |
| F | Fluorine |
| FC | Fluorocarbon |
| FCG | Full concentration gradient |
| Fe | Iron |

| | |
|--------|---|
| FEC | Fluorinated ethylene carbonate |
| FOA | Funding Opportunity Announcements |
| FTE | Full-time equivalent |
| FTIR | Fourier Transform Infrared Spectroscopy |
| FY | Fiscal Year |
| GM | General Motors |
| GREET | Greenhouse Gas, Regulated Emissions, and Energy Use in Transportation |
| HA | Hydrothermal assisted |
| HCMR | High capacity manganese rich |
| HEV | Hybrid Electric Vehicle |
| HF | Hydrofluoric acid |
| HOMO | Highest occupied molecular orbital |
| 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 |
| ICE | Internal combustion engine |
| ICL | Initial capacity loss |
| IE | Ion exchange |
| INL | Idaho National Laboratory |
| IR | Infrared |
| JCESR | Joint Center for Energy Storage Research |
| JCI | Johnson Controls, Inc. |
| kg | Kilogram |
| LBNL | Lawrence Berkeley National Laboratory |
| LCA | Life cycle assessment |
| LCO | Lithium Cobalt Oxide |

| | |
|----------------------------------|--|
| LEESS | Lower-Energy Energy Storage System |
| LFO | Lithium Iron Oxide |
| LFP | Lithium Iron Phosphate |
| Li | Lithium |
| Li ₂ MnO ₃ | Lithiated transition metal oxides |
| Li ₂ ZrO ₃ | Lithium zirconate |
| LIB | Lithium Ion Battery |
| LiBF ₄ | Lithium tetrafluoroborate |
| LiBOB | Lithium bis(oxalate)borate |
| LIBS | Laser-induced breakdown spectroscopy |
| Li-ion | Lithium Ion |
| LiPF ₆ | 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 |
| LOMO | Lowest occupied molecular orbital |
| LT | Low Temperature |
| MD | Machine direction |
| MECT | Mechanical electrochemical-thermal |
| Mg | Magnesium |
| MIT | Massachusetts institute of Technology |
| MLD | Molecular layer deposition |
| Mn | Manganese |
| MOSS | Multi beam optical stress sensor |

| | |
|-------------------|---|
| Mo ₂ C | Molybdenum Carbide |
| MS | Mass spectroscopy |
| NaOH | Sodium hydroxide |
| NCA | Battery cathode material (nickel cobalt aluminum oxide) |
| NCM | Nickel Cobalt Manganese |
| ND | Neutron diffraction |
| NERSC | National Energy Research Scientific Computing Center |
| NDE | Non-Destructive Evaluation |
| Ni | Nickel |
| NMC | Nickel Manganese Cobalt oxide |
| NMP | N-Methylpyrrolidone |
| NMR | Nuclear Magnetic Resonance |
| NREL | National Renewable Energy Laboratory |
| NYBEST | New York Battery and Energy Storage Technology Consortium |
| O ₂ | Oxygen |
| OAS | Open architecture standard |
| OCV | Open-circuit voltage |
| OEM | Original equipment manufacturer |
| ORNL | Oak Ridge National Laboratory |
| P | Phosphorous |
| PAN | Polyacrylonitrile |
| PCA | Principal component analysis |
| PEO | Polyethylene oxide |
| PEV | Plug-in Electric Vehicle |
| PHEV | Plug-In Hybrid Electric Vehicle |
| PI | Principal Investigator |
| PPy | Polypyrrole |
| PVDF | Polyvinylidene difluoride |

| | |
|------------------|---|
| QC | Quality Control |
| R&D | Research and Development |
| RFPI | Request for proposal information |
| ROI | Return on investment |
| RT | Room temperature |
| Ru | Ruthenium |
| S | Sulfur |
| Sb | Antimony |
| SEI | Solid Electrolyte Interface |
| SEM | Scanning Electron Microscope |
| SFG | Sum frequency generation |
| Si | Silicon |
| SIMS | Secondary ion mass spectrometry |
| SiO ₂ | Silicon dioxide |
| SLMP | Stabilized lithium metal powder |
| Sn | Tin |
| SNL | Sandia National Laboratory |
| SOC | State of Charge |
| STEM | Scanning transmission electron microscopy |
| SXAS | Soft X-ray absorption spectroscopy |
| TD | Transverse direction |
| TEM | Transmission Electron Microscope |
| Ti | Titanium |
| TM | Transition Metal |
| TMA | Tri Methyl Aluminum |
| TOF | Time of flight |
| TR-XRD | Time-resolved X-ray diffraction |
| TXM | Transmission x-ray microscope |

| | |
|-------|---|
| USABC | US Advanced Battery Consortium |
| USCAR | U.S. Council for Automotive Research |
| V | Vanadium |
| V | Volts |
| VC | Vinylene Carbonate |
| VIBE | Virtual Integrated Battery Environment |
| VOC | Volatile organic compounds |
| VTO | Vehicle Technologies Office |
| Wh | Watt hour |
| XANES | X-ray Absorption Near Edge Spectroscopy |
| XAS | X-ray Absorption Spectroscopy |
| XPS | X-ray Photoelectron Spectroscopy |
| XRD | X-ray Diffraction (Crystallography) |
| XRF | X-ray Fluorescence |

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