2. Batteries R&D

To strengthen national security, enable future economic growth, support energy dominance, and increase transportation energy affordability for Americans, the Vehicle Technologies Office (VTO) funds early-stage, high-risk research. The research will generate knowledge that industry can advance to deploy innovative energy technologies to support affordable, secure, reliable and efficient transportation systems across America. VTO leverages the unique capabilities and world-class expertise of the national laboratory system and works with partners across industry and academia to develop new innovations in electrification, including advanced battery technologies; advanced combustion engines and fuels, including co-optimized systems; advanced materials for lighter-weight vehicle structures and better powertrains; and energy efficient mobility technologies and systems, including connected and automated vehicles as well as innovations in connected infrastructure for significant systems-level energy efficiency improvement. VTO is uniquely positioned to address early-stage challenges due to its strategic research partnerships with industry (e.g., the U.S. DRIVE and 21st Century Truck Partnerships) that leverage relevant technical and market expertise. These partnerships prevent duplication of effort, focus U.S. Department of Energy (DOE) research on the most critical research and development (R&D) barriers, and accelerate progress. VTO focuses on research that industry either does not have the technical capability to undertake on its own— usually because there is a high degree of scientific or technical uncertainty—or it is too far from market realization to merit sufficient industry emphasis and resources.

The Battery Technologies R&D subprogram funds research programs with partners in academia, national laboratories, and industry, focusing on generating knowledge of high-energy and high-power battery materials and battery systems that can enable industry to significantly reduce the cost, weight, volume and charge time of plug-in electric vehicle (PEV) batteries. The activity supports the development of innovative materials and cell technologies capable of realizing significant cost reductions in two major R&D areas, Advanced Battery Materials R&D, and Advanced Battery Cell R&D. Advanced Battery Materials R&D focuses on early-stage R&D of new lithium (Li)-ion cathode, anode, and electrolyte materials, which account for 50%-70% of PEV battery cost of current technologies. Specifically, this work focuses on the development of new materials that offer a significant improvement in either energy or power and have the potential to achieve the DOE battery cost target of $100/kWh and be capable of charging in 15 minutes or less. Advanced Battery Materials R&D includes the Battery500 research consortium, which is developing “Beyond Li-Ion” technologies. The Battery500 consortium is focusing on designing novel electrode and cell architectures utilizing a Li anode combined with a compatible electrolyte system and high-capacity cathodes and achieving 500 Wh/kg and 1,000 cycles at the lab cell level. R&D also focuses on developing innovative battery materials recycling and reuse technologies to assure sustainability and domestic supply.

The Advanced Battery Cell R&D effort focuses on early-stage R&D of new battery cell technology that contains new materials and electrodes that can reduce the overall battery cost, weight, and volume while improving energy, life, safety, and fast-charging. This R&D area also supports high-fidelity battery performance, life, fast-charging, and safety testing of innovative battery technologies.

Subprogram Feedback

DOE received feedback on the overall technical subprogram areas presented during the 2018 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.

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.

Presentation Number: bat918
Presentation Title: Battery and Electrification R&D Overview
Principal Investigator: Steve Boyd (U.S. Department of Energy)

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

Reviewer 1:
Yes, the program was covered to meet the needs of this reviewer. The material gave a very good overview of the DOE program and goals, and addressed the issues.

Reviewer 2:
The reviewer stated yes, and commented that the speaker did an excellent job of covering all facets of the battery and electrification R&D efforts. Key challenges in each of the main areas of technology and how they were being addressed by ongoing research was discussed. This reviewer reported that the following were covered: Li-ion and non-lithium battery cell development, including new low cobalt (Co) cathode and intermetallic alloy anode work; electric drive developments at higher voltages and lower costs; and grid issues, including fast charging and cybersecurity. A strong case was made for the need to reduce battery cost and charging time, along with the need to reduce cost and increase efficiency of the traction drive system to ensure large market penetration of electric drive vehicles (EDVs). This reviewer commented that concurrent grid infrastructure needs to support widespread acceptance of electric vehicles (EVs) was also addressed. As far as specific technologies are concerned, the presenter did a particularly good job of covering the wide array of outstanding work in the area of power electronics and motors for vehicle electrification.

Reviewer 3:
The reviewer responded positively and explained that battery life must be properly predicted for projects to be funded in the extreme fast charge Li-ion cell area. This reviewer inquired whether it is possible to develop a degradation model of various battery components so that a predictive model is developed, gets shared with stakeholders, and is tested to validate the developed model.

Reviewer 4:
This reviewer indicated yes and suggested the following strategy adjustments: cost of electric vehicle batteries to less than $100/kWh and $6/kW for a 100 kW peak Electric Drive System (EDS); breakout targets by technology areas (e.g., motor, inverter, battery package, controls, and thermal systems); and breakout targets for hybrid electric vehicle (HEV), plug-in hybrid electric vehicle (PHEV), performance EV, and passenger EV.

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

Reviewer 1:
The reviewer responded positively and asserted that there is an excellent balance. The presentation addressed the very near-term 2020 to the longer-term 2030 goals, and provided future roadmap indicators for the technologies being reviewed.

Reviewer 2:
This reviewer stated yes. There is an appropriate balance with all three areas well covered, including nearer-term Li-ion battery development and electric drive research focused on cost reduction; mid-term advanced cell battery, high-voltage electric drive, two-phase cooling, multiphysics integration, and grid integration work; and long-term research on extreme fast charging, new materials development, and cybersecurity,

Reviewer 3:
The reviewer commented that there is a need to make some adjustments. Regarding $6/kW for a 100 kW peak, the reviewer provided the following link to show that HEV sales are slowing (down 19.0%) and strong electric plugged xEVs are increasing (up 46.0%). The reviewer cited an Argonne National Laboratory (ANL) study of

light-duty EDV sales update
(http://www.anl.gov/energy-systems/project/light-duty-electric-drive-vehicles-monthly-sales-updates). With this in mind, the reviewer stated that future targets need to address the higher power requirements for battery, power electronics, and electric drive. Further, this reviewer noted that 100kW is low as a reference point for the future.

Reviewer 4:

This reviewer indicated yes. For wide bandgap (WBG) devices, the reviewer commented that it is necessary to cover voltage range from 48 volt (V) to 1,700V. The reviewer suggested that development of cost and performance optimized silicon carbide (SiC) power package could be one of the long-term (5 years) research goals.

SiC and gallium nitride (GaN) devices are far smaller than Si devices. Therefore, to keep inverter foot-print optimized and smaller, the reviewer explained that it is necessary to have an application-specific integrated circuit for gate driver circuit that should consist primarily of gate driver circuitry, including isolated power supplies and their watchdogs. The reviewer suggested this could be a mid-term goal and could raise the possibility of wide acceptance of SiC and GaN power converter technology for EVs, HEVs, PHEVs, etc.

Question 3: Were important issues and challenges identified?

Reviewer 1:

This reviewer stated yes, and noted that critical issues included cost reduction, power density increases, increased charging speed, grid integration, cybersecurity, and methods to address range anxiety (e.g., longer battery life and improved infrastructure).

Reviewer 2:

In this overview presentation, the reviewer observed several areas were addressed that impact the future of vehicle electrification. Each area had technical issues and challenges that needed to be addressed, which were done to this reviewer’s satisfaction.

Reviewer 3:

The reviewer stated yes, except for how manufacturing will be advanced to support project activities dedicated to achieve 2025 power density and cost targets for electric drive technologies.

Reviewer 4:

This reviewer identified key emerging challenges on the horizon. Firstly, marriage of autonomous with EV means that power management of the low voltage power bus has become safety critical and a challenge in the increased required power for all of the electric actuation and sensing, which could be more than 5kW. Secondly, the reviewer noted that electrical, battery, and component thermal management aspects for extreme fast charging are certainly needed as a future challenge. Finally, this reviewer highlighted the influence of fast charge on graphite (Gr) life, nickel manganese cobalt oxide (NMCxxx), Si, or silicon oxides (SiO_x).

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

Reviewer 1:

The reviewer responded positively and noted that plans to address critical issues and challenges included cooling and multiphysics integration techniques to permit cost reduction and electric drive power density increases. New charger designs and battery cell materials were also proposed for increased charging speed, along with programs to improve grid integration and infrastructure.

Reviewer 2:

This reviewer stated yes, the plans for addressing the issues and challenges associated with the different technologies were identified. The presentation also provided the funding scheduled to support that work. The reviewer further highlighted that one major and key method identified involved forming collaborative teams that included the various labs and industry.

Reviewer 3:

The reviewer remarked that plans were somewhat identified for addressing issues and challenges, and suggested that plans may need minor or major changes as research progresses to achieve 2025 targets.

Reviewer 4:

This reviewer commented to continue U.S.-based WBG based component development—Tesla now has in its Model 3—and suggested this should be supplied and implemented by somehow leveraging overall domestic capability. The reviewer then referenced battery fast charge as related to electrochemistry and thermals. Regarding battery cost, the reviewer noted low cost chemistry (e.g., lithium manganese oxide [LMO]), and suggested to consider funding original equipment manufacturer (OEM) or supplier-based battery cell prototype equipment to speed learning in domestic locations.

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

Reviewer 1:

Progress from last year was somewhat benchmarked against 2016-2017, as indicated by this reviewer. The trend tended toward progress over a larger timeframe that highlighted steady growth based on technology developments.

Reviewer 2:

This reviewer remarked that progress was somewhat clearly benchmarked against the previous year. For example, the reviewer highlighted a very nice chart showing the reduction in battery cost per year, and suggested that adding a full chart of the major accomplishments in the previous year, the current year, and the planned upcoming year would be nice.

Reviewer 3:

The reviewer stated yes, from a budget perspective, but was unsure whether this could be extrapolated to a technology-based progress. The reviewer suggested it might be worthwhile to have a perspective similar to the Advanced Combustion Systems team, which shows progress in emissions, power, power density, and 0-60 miles per hour vehicle performance over time.

Reviewer 4:

This reviewer reported that 2020 and 2025 targets are quite different.

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 key goal of the VTO office, as indicated by this reviewer, is to make electric drive vehicles competitive with fossil fuel powered vehicles in all aspects, particularly performance, cost, and overall life. The reviewer remarked that the projects and plans, as outlined, address the technical issues that need to be overcome to meet those goals.

Reviewer 2:

This reviewer stated yes, the projects in this technology area are all aimed at reducing cost, enhancing performance and efficiency, and improving the driving experience (e.g., increasing range, reliability, and security) to promote widespread EV acceptance and thereby minimize carbon (C) emissions and fossil fuel use.

Reviewer 3:

The reviewer indicated that the projects in this technology area somewhat address the broad problems and barriers that VTO is trying to solve, and noted that projects should have a clear pathway for commercialization.

Reviewer 4:

This reviewer responded yes, generally, and recommended a continued focus to get performance up and cost down. One gap the reviewer identified is the marriage of autonomous with EV, which means that power management of the low voltage power bus has become safety critical and a challenge in the increased required power, Automotive Safety Integrity Level D (ASIL D) safety, and power management for all of the electric actuation and sensing. The reviewer added that the required could be even more than 5kW.

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

Reviewer 1:

The reviewer remarked yes; focus is maintained in the most fruitful areas for research. This reviewer observed excellent management at all levels from Steven Boyd, the Program Manager, who is an exceptional leader, to his experienced and expert team, especially Susan Rogers, who leads the electric drive efforts.

Reviewer 2:

This reviewer agreed that the program area appears to be focused, well-managed, and effective in addressing VTO needs. The reviewer reported that the presentation material outlines the areas that will address current, near-term, and future goals. The material covered areas that are needed on the vehicle side as well as much of the infrastructure concerns.

Reviewer 3:

The reviewer responded positively and commented that, in electric machine R&D work, material properties should be modeled to predict how new material will perform for various mission profiles (tow-speed characteristics) required by EVs, HEVs, PHEVs, etc.

Reviewer 4:

This reviewer asserted that an initiative is needed to attract the new and emerging EV companies to participate and suggested that DOE at least make some focused visits to those new companies to collaborate.

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 expressed that the projects cover a wide range of topics, but are all complementary and focused toward electric vehicle improvement. Projects focused specifically on critical challenges include those related to design, packaging, thermal management, and reliability of innovative chargers and batteries for fast charging and for the grid infrastructure to support them. This reviewer explained that projects were well supported and had a nice balance of innovation and practicality that permitted significant and achievable progress in a reasonable time.

Reviewer 2:

One area that the reviewer identified was the need to have more visible support and/or input from the U.S. Department of Transportation (DOT). That involvement is undoubtedly there, but it was not clearly presented. The work with batteries was a focus of this reviewer, who indicated that the work in that area continues to push the envelope of understanding the issues and resolving them.

Reviewer 3:
This reviewer asserted that cost is key. Although there could be some more detailed trade-off on power density versus cost and manufacturability to meet cost, the reviewer commented that it will continue to lag in adoption without profitable electrification technology.

Reviewer 4:
This reviewer opined that there is too much focus on electric machine technology and little focus on inverter technology. The reviewer advised that attention to battery technology with a clear focus towards commercialization should be given due attention.

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

Reviewer 1:
The reviewer indicated that the projects are novel and represent innovative ways to approach solutions to the issues involved. Further, this reviewer observed a multi-prong collaborative task force with a single mission, using analytical and testing tools from several labs is being used, which is both novel and innovative.

Reviewer 2:
This reviewer stated yes and highlighted some of the more novel approaches: microporous silicon (Si) anodes; Co-free cathodes; fundamental materials characterization of Li cells for extreme fast charging; use of multiphysics for device and package integration; two-phase cooling; and high voltage, WBG power converters.

Reviewer 3:
The reviewer agreed that these projects represent novel and/or innovative ways to approach these barriers. Alternative and variant cooling methods including phase-change cooling related projects should be funded to realize a power-dense air-cooled power converter, which this reviewer asserted will support adoption of the WBG technologies.

Reviewer 4:
Regarding extreme fast charging, this reviewer explained that, perhaps, the critical enabler of 800V max batteries is not so novel or innovative. Of course, the reviewer continued, this then drives needed work in high voltage (HV) power electronics and electric drives.

Question 10: Has the program area engaged appropriate partners?

Reviewer 1:
This reviewer stated yes; each of the projects has identified leaders in the field for collaboration. The level of industrial, academic, and government laboratory interactions in this program is impressive and the partners chosen are recognized experts.

Reviewer 2:
The reviewer responded positively and asserted that vehicle OEMs, battery manufacturers, national laboratories, and parts manufacturers for the battery manufacturers are all involved.

Reviewer 3:
This reviewer opined that industry, university, and DOE lab partnership should be encouraged to solve problems perceived as difficult and/or impossible.

Reviewer 4:
The reviewer commented that, generally, getting major OEMs is key. However, the reviewer indicated that there could be some sort of initiative needed to attract new and emerging EV companies to participate. This reviewer suggested that DOE at least make some focused visits to those new companies to collaborate.

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

Reviewer 1:

The reviewer responded positively and observed regular, arranged meetings with updates that are provided. This reviewer further commented on dynamic direction and support that is delivered based on progress.

Reviewer 2:

This reviewer stated yes and suggested that industry, university, and DOE national laboratory partnerships should be further encouraged to solve problems perceived as difficult and/or impossible.

Reviewer 3:

Generally, the reviewer reported significant evidence of strong collaboration with industry and academia, as well as other government laboratories, though it depends on the project. Each partner is supplying a key appropriate aspect of each project, whether that is new materials, design expertise, modeling expertise, components for test, or facilities.

Reviewer 4:

The reviewer noted a basic model focus on having OEMs and suppliers build functional prototypes. This reviewer also observed labs and universities on materials, basic research, and studies.

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

Reviewer 1:

The reviewer remarked that gaps have been identified, but are a risk level that allows them to exist until the key items are addressed. This reviewer added that the focus has to be on areas that will drive success rather than areas that may have some limited value.

Reviewer 2:

Regarding the design for “Giga-Watt-Hr” (GWh) production of battery cells and packs, this reviewer commented that electrochemistry is important, but will need the balance with manufacturing at large scale to be a factor. Although reducing Co and other materials saves money, so does a more efficient manufacturing technique.

Reviewer 3:

This reviewer indicated that it seems like Li-ion batteries are tracking quite well with the desired trends for cost reduction, as this is happening year after year. In the category of beyond Li-ion projects, there should be some focus to improve Li-Ion technology too; this is needed for large scale adoption of EVs. The reviewer opined that car drivers still have battery reliability in mind when they hit car dealers to buy an EV.

Reviewer 4:

The reviewer recommended other areas to investigate, including the following: three dimensional (3-D) packaging, including additive manufacturing; electro-thermal-mechanical-reliability co-design; high voltage thin film insulators; and new WBG semiconductors (e.g., gallium oxide, diamond).

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

Reviewer 1:

The reviewer asserted that key topics to make this technology reach stated goals are being addressed.

Reviewer 2:

This reviewer commented that future targets need to address the higher power requirements for battery, power electronics, and electric drive, and further highlighted that 100 kW is low as a future reference point.

Reviewer 3:
According to this reviewer, some attention should be given to enabling technologies for inverters, such as packaging material; thermal management materials, including advanced cooling technologies for inverters; inverter interconnects; motor; and connectors, etc.

Reviewer 4:
The reviewer referenced prior comments.

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

Reviewer 1:
This reviewer recommended ensuring state of charge (SOC) and state of health (SOH) algorithms during these events as related to extreme fast charging.

Reviewer 2:
The reviewer suggested other potential areas that may need funding to meet the overall goal of vehicle electrification.

Reviewer 3:
The reviewer commented that eliminating resistive contacts within an inverter and between motor and inverter should be given due consideration. The reviewer explained that, often, Electric Drive (ED) fails or life of ED reduces due to heating of various inter connects within ED system.

Reviewer 4:
This reviewer referenced prior comments.

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

Reviewer 1:
The involvement of the different national laboratories and OEMs has allowed for a multitude of counselors to be involved in evaluating and suggesting all viable approaches that this reviewer could envision.

Reviewer 2:
The program’s current approach was described by this reviewer as well on track.

Reviewer 3:
This reviewer was unable to offer any quality ideas.

Reviewer 4:
The reviewer remarked that capturing requirements early should be encouraged for each project. Further, this reviewer suggested accomplishing this by identifying a specific application of underlying technology being developed through DOE-VTO funding. Often, R&D work goes somewhat satisfactorily; however, research faces the valley of death due to lack of adoption when research outcomes fall short in addressing application needs. The reviewer opined that this can be addressed by encouraging industry partnership with a commitment to demonstrating technology in an identified application.

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

Reviewer 1:
The reviewer commented that this presentation did exactly what was needed—it gave a very good overview of the programs involved, their tasks, goals, and accomplishments. This presentation was also effective as it highlighted some of the key issues that must be overcome.

Reviewer 2:
The reviewer stated none.

Reviewer 3:
Continuing focus on the most critical constraints to a widespread market penetration of electric vehicles (i.e., cost, range, and reliability) was recommended by this reviewer.

Reviewer 4:
This reviewer suggested that increased involvement of industry reviewers should be considered during selection of projects for DOE-VTO funding. If possible, university and DOE national laboratory projects should have industry advisors with application oriented mindsets. Otherwise, continued this reviewer, DOE-VTO funded R&D work runs the risk of falling into the valley of death.

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.

Table 2-1—Project Feedback

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat049	Tailoring Integrated Layered- and Spinel Electrode Structures for High-Capacity Lithium-Ion Cells †	Michael Thackery (ANL)	2-19	3.33	3.17	3.50	3.17	**3.25**
bat052	Design of High-Performance, High-Energy Cathode Materials †	Marca Doeff (LBNL)	2-22	3.17	3.17	3.33	2.83	**3.15**
bat056	Development of High-Energy Cathode Materials †	Jason Zhang (PNNL)	2-25	3.50	3.17	3.50	2.67	**3.23**
bat085	Interfacial Processes—Diagnostics †	Robert Kostecki (LBNL)	2-29	3.40	3.40	3.40	3.50	**3.41**
bat106	High-Capacity, Multi-Lithium Oxide Cathodes and Oxygen Stability †	Jagit Nanda (ORNL)	2-34	3.17	3.00	3.17	3.33	**3.10**
bat164	Thick, Low-Cost, High-Power Lithium-Ion Electrodes via Aqueous Processing †	Jianlin Li (ORNL)	2-37	3.75	3.75	3.50	3.00	**3.63**
bat168	Process Development and Scale-Up of Critical Battery Materials—Continuous Flow-Produced Materials	Krzysztof Pupek (ANL)	2-39	3.17	3.33	3.33	3.33	**3.29**
bat183	In Situ Solvo-Thermal Synthesis of Novel High-Capacity Cathodes †	Feng Wang (BNL)	2-42	3.33	3.33	3.67	3.33	**3.38**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat220	Addressing Heterogeneity in Electrode Fabrication Processes †	Dean Wheeler (Brigham Young U.)	2-45	3.67	3.33	3.33	3.33	**3.42**
bat230	Nanostructed Design of Sulfur Cathode for High Energy Lithium-Sulfur Batteries †	Yi Cui (Stanford University)	2-48	3.70	3.50	3.40	3.40	**3.53**
bat232	High Energy Density Electrodes via Modifications to the Inactive Components and Processing Conditions †	Vincent Battaglia (LBNL)	2-53	3.00	3.00	3.25	3.00	**3.03**
bat235	Characterization Studies of High-Capacity Composite Electrode Structures †	Jason Croy (ANL)	2-55	3.50	3.33	3.50	3.00	**3.35**
bat240	High-Energy Anode Material Development for Lithium-Ion Batteries, Cary Hayner, Sinode Systems †	Cary Hayner (Sinode Systems)	2-58	3.13	2.88	3.50	2.67	**2.99**
bat241	Advanced High-Performance Batteries for Electric Vehicle (EV) Applications †	Ionel Stefan (Amprius)	2-61	3.38	3.63	2.50	3.25	**3.38**
bat247	High-Energy Lithium Batteries for Electric Vehicles †	Herman Lopez (Envia Systems)	2-64	3.13	3.38	3.25	2.83	**3.23**
bat252	Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Electrochemistry and Evaluation	Daniel Abraham (ANL)	2-67	3.33	3.33	3.33	3.33	**3.33**
bat253	Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Theory and Modeling	Hakim Iddir (ANL)	2-70	3.67	3.67	3.67	3.50	**3.65**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat254	Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Materials Characterization	John Vaughey (ANL)	2-73	3.33	3.33	3.50	3.17	**3.33**
bat263	Electrodeposition for Low-Cost, Water-Based Electrode Manufacturing †	Stuart Hellring (PPG Industries)	2-76	3.17	3.33	3.17	3.17	**3.25**
bat264	Lithium-Ion Battery Anodes from Electrospun Nanoparticles/Conducting Polymer Nanofibers †	Peter Pintauro (Vanderbilt U.)	2-79	3.50	3.17	3.00	3.00	**3.21**
bat266	Co-Extrusion (CoEx) for Cost Reduction of Advanced High-Energy and High-Power Battery Electrode Manufacturing †	Ranjeet Rao (PARC)	2-82	3.50	3.00	3.33	3.00	**3.17**
bat269	An Integrated Flame-Spray Process for Low-Cost Production of Battery Materials †	Chad Xing (U. of Missouri)	2-85	3.00	2.33	3.00	2.67	**2.63**
bat273	Composite Electrolyte to Stabilize Metallic Lithium Anodes †	Nancy Dudney (ORNL)	2-88	3.00	3.13	3.13	3.00	**3.08**
bat282	Development of High-Energy Lithium-Sulfur Batteries †	Jun Liu (PNNL)	2-92	3.50	3.30	3.40	3.13	**3.34**
bat293	A Closed-Loop Process for End-of-Life Electric Vehicle Lithium-Ion Batteries †	Yan Wang (WPI)	2-96	3.38	3.63	3.50	3.33	**3.51**
bat296	Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries †	Chulheung Bae (Ford)	2-99	3.40	3.50	3.70	3.40	**3.49**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat298	Efficient Simulation and Abuse Modeling of Mechanical-Electrochemical-Thermal Phenomena in Lithium-Ion Batteries †	Shriram Santhanagop-alan (NREL)	2-103	3.50	3.60	3.60	3.40	**3.55**
bat299	Microstructure Characterization and Modeling for Improved Electrode Design †	Kandler Smith (NREL)	2-108	3.70	3.70	3.50	3.63	**3.67**
bat300	Enhancement and Deployment of VIBE, the Open Architecture Software (OAS) Environment †	Srikanth Allu (ORNL)	2-113	3.60	3.50	3.60	3.40	**3.53**
bat301	Experiments and Models for the Mechanical Behavior of Battery Materials †	Sergiy Kalnaus (ORNL)	2-117	3.50	3.50	3.40	3.50	**3.49**
bat302	Microstructure Imaging and Electrolyte Transport Property Measurements for Mathematical Modeling †	Venkat Srinivasan (ANL)	2-121	3.40	3.20	3.50	3.30	**3.30**
bat303	Exploring How Electrode Structure Affects Electrode-Scale Properties Using 3-D Mesoscale Simulations †	Scott Roberts (SNL)	2-125	3.50	3.50	3.40	3.60	**3.50**
bat307	Discovery of High-Energy Lithium-Ion Battery Materials †	Wei Tong (LBNL)	2-129	3.17	3.33	3.33	3.00	**3.25**
bat310	Advancing Solid-State Interfaces in Lithium-Ion Batteries †	Nenad Markovic (ANL)	2-132	3.30	3.20	3.30	3.00	**3.21**
bat312	Advanced Lithium-Ion Battery Technology: High-Voltage Electrolyte †	Joe Sunstrom (Daikin)	2-136	3.10	3.20	2.80	3.00	**3.10**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat319	Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte †	Shirley Meng (UC-San Diego)	2-140	3.70	3.30	3.40	3.30	**3.41**
bat321	Solid-State Inorganic Nanofiber Network-Polymer Composite Electrolytes for Lithium Batteries †	Nianqiang Wu (West Virginia U.)	2-144	3.60	3.40	3.20	3.30	**3.41**
bat322	High Conductivity and Flexible Hybrid Solid-State Electrolyte †	Eric Wachsman (U. of Maryland)	2-149	3.30	3.50	3.50	3.30	**3.43**
bat323	Self-Forming Thin Interphases and Electrodes Enabling 3-D Structured High Energy Density Batteries †	Glenn Amatucci (Rutgers U.)	2-153	3.50	3.50	3.10	3.50	**3.45**
bat326	Self-Assembling and Self-Healing Rechargeable Lithium Batteries †	Yet Chiang-Ming (MIT)	2-158	3.40	3.30	3.50	3.50	**3.38**
bat328	Dendrite-Growth Morphology Modeling in Liquid and Solid Electrolytes †	Yue Qi (Michigan State U.)	2-163	3.60	3.60	3.50	3.70	**3.60**
bat329	Understanding and Strategies for Controlled Interfacial Phenomena in Lithium-Ion Batteries and Beyond †	Perla Balbuena (Texas A&M U.)	2-168	3.40	3.30	3.70	3.40	**3.39**
bat330	Electrochemically Responsive, Self-Formed, Lithium-Ion Conductors for High-Performance Lithium-Metal Anodes †	Donghai Wang (Penn State U.)	2-173	3.50	3.30	3.30	3.40	**3.36**
bat332	High Electrode Loading Electric Vehicle Cell †	Mohamed Taggougui (24M Technologies)	2-177	3.63	3.63	3.25	3.13	**3.52**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat344	Electrolyte Reactivity and Its Implication for Solid-Electrolyte Interface (SEI) Formation	Kristin Persson (LBNL)	2-180	3.42	3.58	3.58	3.33	**3.51**
bat345	Chemical Reactivity of Silicon at the Surface	Gabe Veith (ORNL)	2-185	3.42	3.42	3.58	3.25	**3.42**
bat346	Spectroelectrochemistry of Silicon Model Electrodes	Robert Kostecki (LBNL)	2-190	3.58	3.67	3.50	3.33	**3.58**
bat347	Surface Analysis of the Silicon Solid-Electrolyte Interface (SEI)	Chunmei Ban (NREL)	2-194	3.33	3.33	3.33	3.17	**3.31**
bat348	Synthesis and Stability of Lithium Silicate and Its Interaction with the Solid-Electrolyte Interface (SEI)	Chris Apblett (SNL)	2-194	3.25	3.08	3.25	3.33	**3.18**
bat349	Research Facilities Support	Kyle Fenton (SNL)	2-204	3.33	3.42	3.50	2.50	**3.29**
bat350	Electrode Characterization and Analysis	Daniel Abraham (ANL)	2-209	3.25	3.50	3.63	3.25	**3.42**
bat351	Active Particle Studies	Baris Key (ANL)	2-212	3.38	3.25	3.38	3.13	**3.28**
bat352	Active Materials Advancements	Zhengcheng Zhang (John) (ANL)	2-215	3.38	3.38	3.63	3.13	**3.38**
bat353	Crucial Supporting Materials Advancements	Gao Liu (LBNL)	2-218	3.50	3.25	3.38	3.38	**3.34**
bat355	Development of High-Performance Lithium-Ion Cell Technology for Electric Vehicle Applications †	Keith Kepler (Farasis Energy)	2-221	3.33	3.50	3.83	3.33	**3.48**
bat356	Lithium-Ion Cell Manufacturing Using Directly Recycled Active Materials †	Mike Slater (Farasis Energy)	2-225	3.50	3.50	3.50	3.33	**3.48**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat357	Thicker Cathode Coatings for Lithium-Ion Electric Vehicle Batteries †	Stuart Hellring (PPG Industries)	2-228	3.33	3.33	3.50	3.33	**3.35**
bat358	Advanced Separators for Vehicle Lithium Battery Applications †	Junqing Ma (Celgard)	2-231	3.00	2.67	3.33	2.83	**2.85**
bat359	Status and Challenges of Electrode Materials for High Energy Cells	Stanley Whittingham (Binghamton U.)	2-234	3.60	3.40	3.60	3.40	**3.48**
bat360	Overview and Synthesis of High-Nickel Nickel Manganese Cobalt Oxide (NMC) Cathodes	Arumugam Manthiram (UT-Austin)	2-239	3.70	3.80	3.60	3.60	**3.73**
bat361	Lithium-Sulfur Batteries: From Materials Understanding to Device Integration	Yi Cui (Stanford University)	2-243	3.42	3.67	3.67	3.50	**3.58**
bat362	Lithium-Metal Anodes: Problems and Multiple Solutions Based on Hosts, Interphase, and Electrolytes	Jun Liu (PNNL)	2-247	3.90	3.90	3.80	3.70	**3.86**
bat363	Understanding Performance Limitations in Thick Electrodes, Ping Liu	Ping Liu (UC-San Diego)	2-251	3.40	3.30	3.40	3.20	**3.33**
bat364	Coatings for Cathode and Separator	Jihui Yang (U. of Washington)	2-255	3.50	3.70	3.50	3.50	**3.60**
bat365	Stabilizing Lithium-Metal Anode by Interfacial Layer	Zhenan Bao (Stanford University/ SLAC)	2-260	3.30	3.40	3.20	3.20	**3.33**
bat366	Advanced Imaging and Spectroscopic Study of Electrochemically Deposited Lithium Metal	Shirley Meng (UC-San Diego)	2-264	3.60	3.50	3.60	3.30	**3.51**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat367	Integrated Characterization Studies of Battery500 Consortium	Xiao Yang-Qing (BNL)	2-269	3.60	3.60	3.50	3.50	**3.58**
bat368	Battery500 Integrated Cell Diagnostics and Modeling to Identify Critical Gaps in Achieving High Cycle Life	Eric Dufek (INL)	2-274	3.25	3.13	3.25	3.00	**3.16**
bat369	High Energy Rechargeable Lithium-Metal Cells: Fabrication and Integration	Jie Xiao (PNNL)	2-278	3.60	3.30	3.60	3.40	**3.43**
bat370	Advanced Diagnostics of Nickel-Rich, Layered-Oxide Secondary Particles	Chueh, William C. (Stanford University/ SLAC)	2-283	3.38	3.38	3.13	3.25	**3.33**
Overall Average				**3.42**	**3.39**	**3.42**	**3.27**	**3.39**

† Denotes a poster presentation.

Presentation Number: bat049
Presentation Title: Tailoring Integrated Layered and Spinel Electrode Structures for High-Capacity Lithium-Ion Cells
Principal Investigator: Michael Thackery (Argonne National Laboratory)

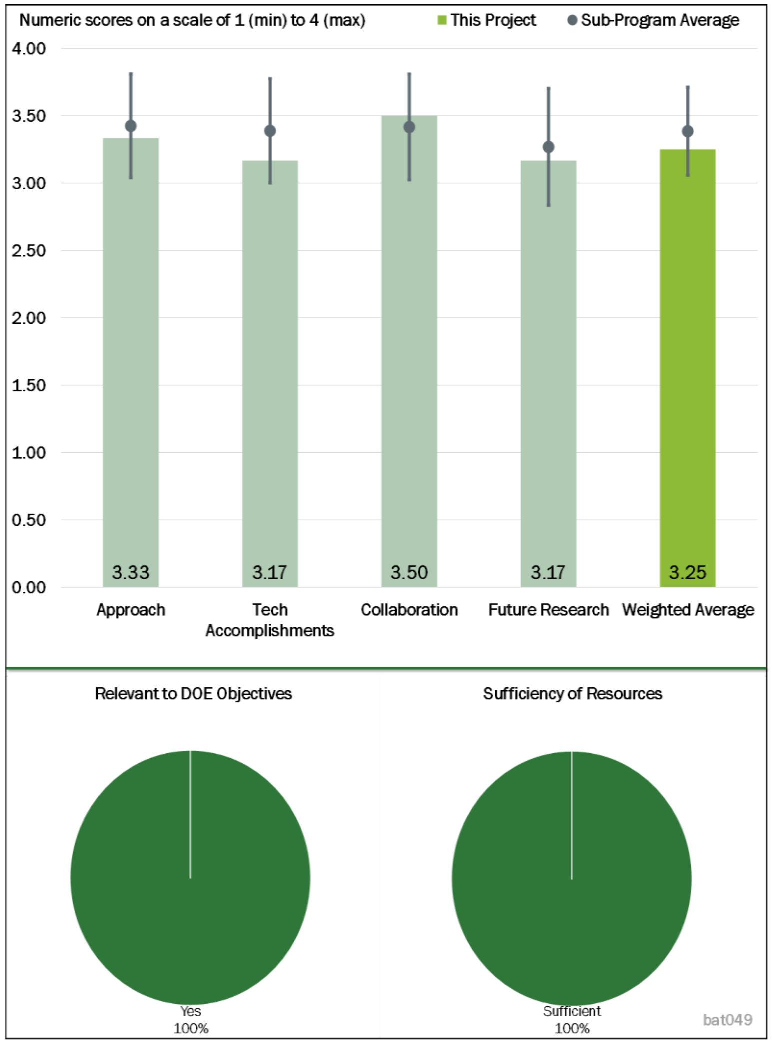

Figure 2-1 - Presentation Number: bat049 Presentation Title: Tailoring Integrated Layered and Spinel Electrode Structures for High-Capacity Lithium-Ion Cells Principal Investigator: Michael Thackery (Argonne National Laboratory)

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 and well-planned.

Reviewer 1:
The reviewer stated that the project team reported the approaches and results of the optimization of cathode material, manganese (Mn)-rich layered-layered-spinel (LLS). The reviewer remarked that the potential merits of high capacity (high energy density) and low-cost have been demonstrated. The reviewer said that the stabilizing surface treatment with the approaches of chemical modification, novel electrolyte, etc., has been successfully addressed. The reviewer remarked that excellent progress has been made in designing the new cathode materials.

Reviewer 2:
The reviewer stated that the project optimizes the performance of structurally-integrated "composite" electrode structures with a prime focus on LLS materials and designs effective strategies to mitigate surface degradation of integrated structures to improve and maintain their stability and rate capability when charged to high potentials [i.e., 4.5V to 4.6V]. The reviewer also noted that this project aims to enable high first-cycle efficiencies, enhanced rate performance, and relative stability.

Reviewer 3:
The reviewer expressed that this project has a generally good approach to the discovery and validation of LLS cathode materials. The reviewer stated that based on the history of the project team, the reviewer is confident in the quality of the work that underlies this project, but pointed out that the project's research summary slides are relatively vague (i.e., on the surface modification and the role of electrolytes on stability). The reviewer would have appreciated additional explanation into the materials synthesis methods and the selection of LLS

compositions or modifications. During a discussion between the reviewer and the project team during the poster session, it was made clear that the spinel is meant to stabilize the structure. The reviewer further noted, however, the distribution and integration of the spinel is quite challenging and may not be controllable enough to achieve appropriate synthetic scale-up. The reviewer said the application of surface stabilization strategies (i.e., with alumina or other coatings) and electrolyte optimization is warranted and, as the results show, effective.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that a new Mn-rich LLS was proposed. The reviewer remarked that technical approaches to address the challenge of capacity fading have been successfully performed, and that significant progress has been made since the last review meeting.

Reviewer 2:

The reviewer stated that this project has made good progress towards developing strategies to improve the performance of LLS cathodes. The reviewer also noted that standard strategies of thermal treatments, electrolyte optimization, and particle coating are implemented to assist in the stability of the particles. The reviewer pointed out that the extra stabilization strategies seem to compensate for known degradation mechanisms of the LLS including the dissolution of Mn. The reviewer commented that for future reference, a state-of-the-art cathode material such as NMC-622 or NMC-811 should be used to demonstrate the benefit of these materials to energy density, rather than using NMC-532, despite NMC-532 being closer in stoichiometry to the LLS.

Reviewer 3:

The reviewer observed that this project develops Mn-rich LLS composition and that the first-cycle efficiency is approximately 95%. The reviewer stated that small-scale testing against NMC-532 cathodes shows that the LLS materials are promising options. The reviewer noted that the project team is using lithium titanate (LTO) as the anode mitigates deleterious side reaction. The reviewer also noted that testing of LLS baseline in LLS//LTO configurations verifies stability of cathode to Li extraction and insertion where the LLS is the source of Li. The reviewer commented that about 350 cycles of approximately 180 milliampere-hours/gram (mAh/g), 4.45V Li/ lithium ion (Li+) achieved in LLS//LTO coin cells before around a 20% loss. The reviewer noted that the project team found critical surface issues and that the project team did the chemical modification/electrolyte study to stabilize the surface. The reviewer summarized that about 800 (Watt-hours per kilogram oxide (Wh/kg_{oxide}) was demonstrated for 100 cycles to 4.5V. However, the project team needs to demonstrate bigger cell performance and check if LTO has any gassing issue.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted that a team at ANL leads the work and there is collaboration among seven total partners. The reviewer stated that multiple research results were achieved through the collaborative work, such as stabilization of material surface with electrolytes and full cell test.

Reviewer 2:

The reviewer remarked that the collaboration across the project team appears effective. The reviewer also stated that there is a dearth of information as to which collaborator provides what project work.

Reviewer 3:

The reviewer noted that the project team works with different teams at ANL, Northwestern University, and Oak Ridge National Laboratory (ORNL).

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

Reviewer 1:

The reviewer said that the future project plan utilizes standard strategies for addressing particle and electrode stability, but it is somewhat vague. The reviewer would like to see greater focus on the effect of spinel integration, including synthetic conditions, on cycle life, and its stability within the LLS structure.

Reviewer 2:

The reviewer suggested more detailed cost analysis to compare with NMC-532 and to provide more evidence that this is a low-cost cathode material. The reviewer also suggested that future work to add to the understanding of the capacity fading mechanism of the large pouch cell with this new cathode material, so that the continued improvements can be addressed.

Reviewer 3:

The reviewer remarked that the proposed future work is in a logical manner.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer summarized that the DOE objectives require the cathode materials to be high safety, high energy density, and low cost. The reviewer noted that the Mn-rich LLS cathode material potentially matches well with DOE targets.

Reviewer 2:

The reviewer noted that that the project goal was to synthesize and stabilize LLS structures that could meet DOE energy density and cycle life goals. The reviewer confirmed that least in theory, this strategy could achieve cathode capacities that are competitive or greater than the state-of-the-art, but they require additional development—particularly to achieve cycle lifetimes that are industrially relevant.

Reviewer 3:

The reviewer remarked that the Mn-rich electrodes are being developed in order to realize competitive alternatives to nickel (Ni)/Co-rich chemistries. The reviewer stated the three-component, Mn-rich, “LLS” composite cathodes have been designed that show competitive oxide energies as compared with an industrial NMC-532. The reviewer commented that combined approaches of new surface materials and electrolyte formulations have demonstrated approximately 800 Wh/kg oxide energy densities in full-cell configurations using Gr anodes.

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 is led by ANL and parted with CNM, Northwestern University, ORNL, and others. The reviewer said the resources provide sufficient capabilities of synthesis, analysis, and evaluation.

Reviewer 2:

The reviewer stated that the resources are sufficient for the project.

Reviewer 3:

The reviewer noted that the project achieved one milestone and that the other two milestones are close to complete and ongoing.

Presentation Number: bat052
Presentation Title: Design of High-Performance, High-Energy Cathode Materials
Principal Investigator: Marca Doeff (Lawrence Berkeley National Laboratory)

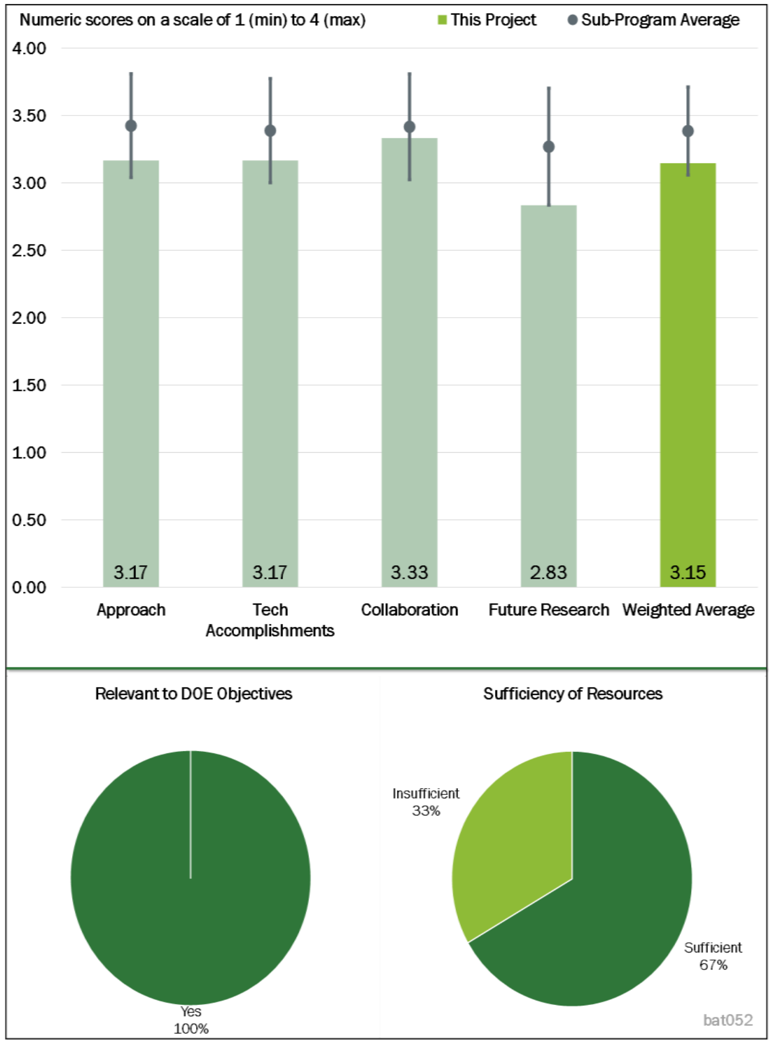

Figure 2-2 - Presentation Number: bat052 Presentation Title: Design of High-Performance, High-Energy Cathode Materials Principal Investigator: Marca Doeff (Lawrence Berkeley National Laboratory)

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 and well-planned.

Reviewer 1:

The reviewer remarked that high-Ni NMCs have been considered as the promising cathode materials for Li-ion batteries; however, their thermal stability and structural evolution has not been fully understood. The reviewer stated that the project team used several advanced techniques to understand those fundamental issues.

Reviewer 2:

The reviewer stated that the present work uses synchrotron techniques and microscopy to understand thermal and high voltage cycling behavior of NMCs. The reviewer noted that the project team used this information to develop strategies to improve behavior and understand the effects. The reviewer said the go/no-go decision is focused on core-shell composites made by spray pyrolysis. The reviewer commented that the project team will explore alternative synthesis approaches.

Reviewer 3:

The reviewer stated that the degree of characterization of NMC chemistry is very thorough, particularly related to the effects of de-lithiation and high temperature. The reviewer noted that experiments that compare surface versus bulk states are particularly valuable (e.g., full-field transmission X-ray microscope [TXM] mapping of Ni content and soft X-ray absorption spectroscopy [XAS]). The reviewer commented that in previous years, the project has looked at the differences between chemical and electrochemical lithiation, finding some discrepancy in surface reconstruction. The reviewer remarked that this year, most work appears to have been conducted on chemically de-lithiated samples, so there remains some question about the relevance of these surface studies to application in a practical format. The reviewer also stated that the goals of this project are to develop high-energy and long cycle life cathode materials, and there have been no performance studies executed this year to emphasize the relevance of the microscale materials transformations. The reviewer asked about the relevance of studying thermal behavior at temperatures as high, or higher than, 250° Celsius (C) and stated these temperatures are unlikely in battery cell environments. The reviewer remarked that although these findings are admirable as a fundamental study of thermodynamics and kinetics, there is little connection between the phenomena studied and design criteria for more robust cathode materials.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer stated that the project team has applied both ex situ and in situ techniques of X-ray powder diffraction (XRD), XAS, soft XAS, and transmission electron microscopy (TEM) to understand the structural evolution of NMCs, which is very important design reliable method to stabilize those cathode materials in a de-lithiated state.

Reviewer 2:

The reviewer remarked that this project studied NMC-622 and NMC-811 chemical de-lithiation, performed NMC-622 and NMC-811 in situ heating experiments, compared bulk thermal stabilities, etc. The reviewer noted that the project team found the thermal stability decreases as Li decreases and Ni rises. The reviewer remarked that the surface sensitive techniques reveal a more complex behavior than the bulk techniques of XAS and XRD.

Reviewer 3:

The reviewer said, as usual from the project team, the wealth of data and thoroughness of the characterization is excellent. However, because the goal of the project is to provide insight into the performance of NMCs, it is unfortunate that no electrochemical results are shown. Furthermore, the objectives mention high voltage behavior and variants of NMC materials in doped or graded compositions, but there were no results on these. The reviewer commented that because this project ends this year, the reviewer would have liked to see experimental progress on the design of more robust NMC materials.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted that the project team worked with Stanford Synchrotron Radiation Lightsource (SSRL) and Brookhaven National Laboratory (BNL).

Reviewer 2:

The reviewer stated that the extensive and varied characterization results emphasize that there is a strong collaborative aspect to this project. The reviewer noted that however, there is not enough explanation of the particular contributions of individual project collaborators.

Reviewer 3:

This work was collaborated within several groups in Lawrence Berkeley National Laboratory (LBNL) and BNL. The reviewer did not see how much the contribution from each group was to finish this work.

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

Reviewer 1:

The reviewer commented that for the rest of fiscal year (FY) 2018, the project team will finish up the thermal characterization of NMC-811 and investigate the effects of titanium (Ti)-substitution on phase behavior, thermal stability, and electrochemical behavior. The reviewer noted that new proposals for work on cathode materials and Na-ion battery materials are being prepared now.

Reviewer 2:

The reviewer stated that the project is near completion, but several objectives have yet to be met. The reviewer said that continuing the current studies with the Ti-substituted material and finishing the analysis of thermal treatment with the same methods should be sufficient.

Reviewer 3:

The reviewer remarked that the project team proposed to finish up the thermal characterization of NMC-811 and Ti-substituted NMCs. The reviewer also believed this direction is important and should be continued. The reviewer remarked that the research of the sodium (Na)-ion is not very interesting, as this battery system would offer higher energy density and cannot be used in EVs, at least in the near future.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said obtaining a fundamental understanding of material transformations in NMCs is very supportive of DOE goals.

Reviewer 2:

The reviewer expressed that Ni-rich NMCs are key cathode materials for high-performance Li-ion batteries. The reviewer said this project provides further understanding of the structural evolution of those cathode materials under a de-lithiated state, which is very important to improve the design of robust electrode materials.

Reviewer 3:

The reviewer commented that the presented work demonstrates the trend (layered→ disordered→spinel→M_3O_4→spinel→MO (rock salt) as the temperature is raised. The reviewer said surface sensitive techniques reveal a more complex behavior than the bulk techniques of XAS and XRD.

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 this research and this project applied many advanced techniques, such as in situ or ex situ XRD, XAS, soft XAS, and TEM, to perform the fundamental study.

Reviewer 2:

The reviewer commented that given this project is close to the end, the project team only completed four out of eight milestones. The reviewer said the project's no-go decision was on core-shell composites made by spray pyrolysis.

Reviewer 3:

The reviewer said that the resources are sufficient, but could be better utilized to focus on material performance and the design of new robust cathode materials.

Presentation Number: bat056
Presentation Title: Development of High-Energy Cathode Materials
Principal Investigator: Jason Zhang (Pacific Northwest National Laboratory)

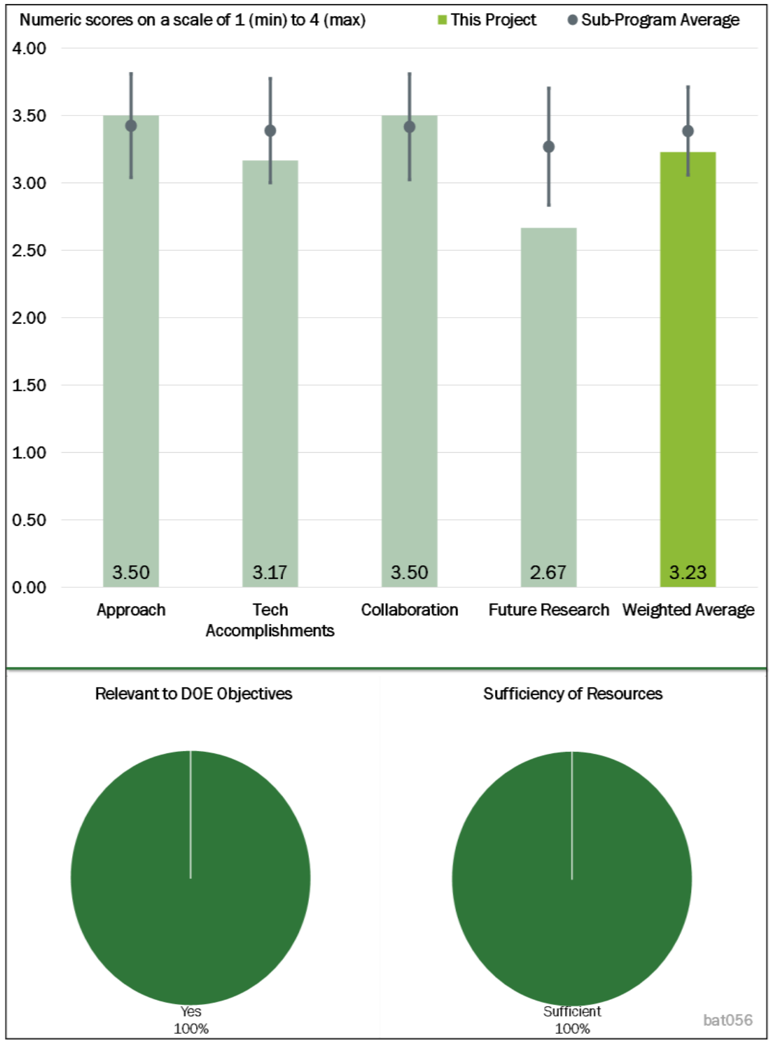

Figure 2-3 - Presentation Number: bat056 Presentation Title: Development of High-Energy Cathode Materials Principal Investigator: Jason Zhang (Pacific Northwest National Laboratory)

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 and well-planned.

Reviewer 1:

The reviewer remarked that high-Ni NMCs have been demonstrated as high-energy density cathode materials for next-generation Li+ batteries. The reviewer noted that the fast capacity fading has been one of the key barriers to commercialize those electrode materials. The reviewer commented that the project team applied different synthetic approaches to address those technical difficulties and showed very impressive improvement.

Reviewer 2:

The reviewer remarked that the technical approach to this project is straightforward and individual efforts complement each other nicely. The reviewer commented, at first, the project team synthesizes high Ni NMC materials and evaluates the importance of annealing temperature on primary particle size. The reviewer noted that using primarily electrochemical methods and microscopy, intraparticle cracking is found to be a factor in cycle life degradation—as discussed in the community at large over the past few years. The reviewer said this issue is tackled by evaluating an optimized electrolyte formulation, and by doping of particles with aluminum (Al) or zirconium (Zr). The reviewer commented that both methods are somewhat successful in limiting cracking of secondary particles, and characterizing their effects on performance is thorough. The reviewer stated that while progress has been good, additional analysis of materials using chemical methods such as spectroscopic or diffraction to understand interface structure would benefit this work.

Reviewer 3:

The reviewer stated that this project uses a co-precipitation method to synthesize the Ni-rich NMC cathode with different compositions and employs the optimized electrolyte and additive to enhance the cycling performance and electrode and electrolyte interface stability. The reviewer remarked that the project team optimized the doping elements and did the surface treatment to enhance the stability of Ni-rich NMC cathode materials. In addition, the project team applied advanced techniques to investigate the capacity improvement mechanism of solid electrolyte surface modification. The reviewer noted that although improved performance of Ni-rich NMC cathodes can be achieved in coin cells, their performance in Gr and NMC pouch cells still need to be further studied.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that this project improved the cycling performance and the interface stability of NMC cathode by using a novel additive. The reviewer remarked that the project team used an optimized electrolyte to achieve excellent 500 cycling performance of NMC cathode and Al doping to enhance the NMC cathode and electrolyte interface stability. In addition, the project team combined uniform coating and a novel additive to enhance the cycling stability of the NMC cathode. The reviewer cautioned that the project team needs to demonstrate Ni-rich NMC performance to reach 200 mAh/g and 80% capacity retention after 300 cycles by the end of the program.

Reviewer 2:

The reviewer noted the report discussed the effects of the electrolyte, Al doping and zirconium dioxide (ZrO_2) coating. However, the reviewer suggested a systematic study, which means the optimization of each parameter is critical for fully understanding the function of every approach.

Reviewer 3:

The reviewer remarked that the project is focused and the results are clearly beneficial to understanding degradation mechanisms in high-Ni NMCs, as well as mitigation strategies. The reviewer said the selection of a non-commercial NMC stoichiometry of NMC-76 is alright, but using a formulation closer to state-of-the-art NMC-811 would be better. The reviewer also believed this project could be more ambitious in its objectives toward a fundamental understanding of interface degradation of high-Ni-NMCs. The reviewer said, particularly, there are other mechanisms beyond particle cracking that are known to lead to capacity fade, including gassing at high voltages and cathode-electrolyte interphase (CEI) instability. The reviewer noted that investigating Al and Zr doping is interesting, but a better understanding of why we would use either Zr, Al, or other dopants (i.e., atomic size, valence, etc.) would aid in the design of more stable materials.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer pointed out this work is led by Pacific Northwest National Laboratory (PNNL) and collaborated among several partners from ANL, BNL, etc. The reviewer remarked the collaboration is excellent.

Reviewer 2:

The reviewer said collaboration among the team appears strong; however, individual collaborator contributions are not explicitly noted.

Reviewer 3:

The reviewer noted that ANL provides standard NMC cathode and materials for testing, Missouri University of Science and Technology is doing atomic layer deposition (ALD) coating, BNL performs in situ XRD on electrode materials, and Army Research Laboratory (ARL) is studying electrolytes and additives.

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

Reviewer 1:

The reviewer suggested that the project team should also work on optimizing doping and coating. The reviewer also suggested that the project team work on understanding how much doping is needed for the best performance. The reviewer also suggested working to determining what the thickness of the coating yields the best performance.

Reviewer 2:

The reviewer cautioned that developing a low-cost coating process could be a big project, and given this project is too close to the end date (September 2018), the reviewer did not believe this can be done by the end of program.

Reviewer 3:

The reviewer commented that this project needs to better define how to identity electrolyte additives for better interface stability. The reviewer said a fundamental study of CEI structure for high-Ni NMCs is important, but the suggestion of spatially resolved energy dispersive X-ray spectroscopy (EDS) will not provide a comprehensive picture to accomplish this goal. The reviewer remarked that developing a low-cost coating process is not an ideal goal for a national laboratory project, particularly because there are already advanced efforts in industry to accomplish this. The reviewer commented that a partnership with a material supplier or company that specializes in ALD coating might be preferred. The reviewer noted that a study of pouch cell configurations to validate results from coin cells is an excellent idea.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

This reviewer expressed that this project supports DOE objectives toward higher energy cathode materials and lower Co contents. The reviewer said that by understanding degradation mechanisms and mitigation strategies, we can guide the design of more robust materials.

Reviewer 2:

The reviewer remarked that high-Ni NMCs offer high energy density and that this is consistent with the overall DOE objective.

Reviewer 3:

The reviewer said the work presented demonstrates a long cycle life, especially the optimized electrolyte. The reviewer noted the ability to achieve 1,000 cycles for 80.6% of cycling with the Li//NMC-76 cell under high voltage (greater than 4.5V) is great.

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 partners applied the sufficient resources to optimize the high-Ni NMCs and achieve the plan in a timely fashion.

Reviewer 2:

The reviewer said that given the scope of the project, that the resources are sufficient.

Reviewer 3:

The reviewer stated the project optimized Ni-rich NMC cathode materials using a controlled co-precipitation method, and improved the cycling stability of NMC-76 cathode materials with optimized electrolyte and additives and/or a surface engineering modification. The reviewer remarked that the project team identified a surface lattice doping effect on the cycling stability of NMC-76 at high charge cut off voltage. The reviewer noted that three out of four milestones were met.

Presentation Number: bat085
Presentation Title: Interfacial Processes—Diagnostics
Principal Investigator: Robert Kostecki (Lawrence Berkeley National Laboratory)

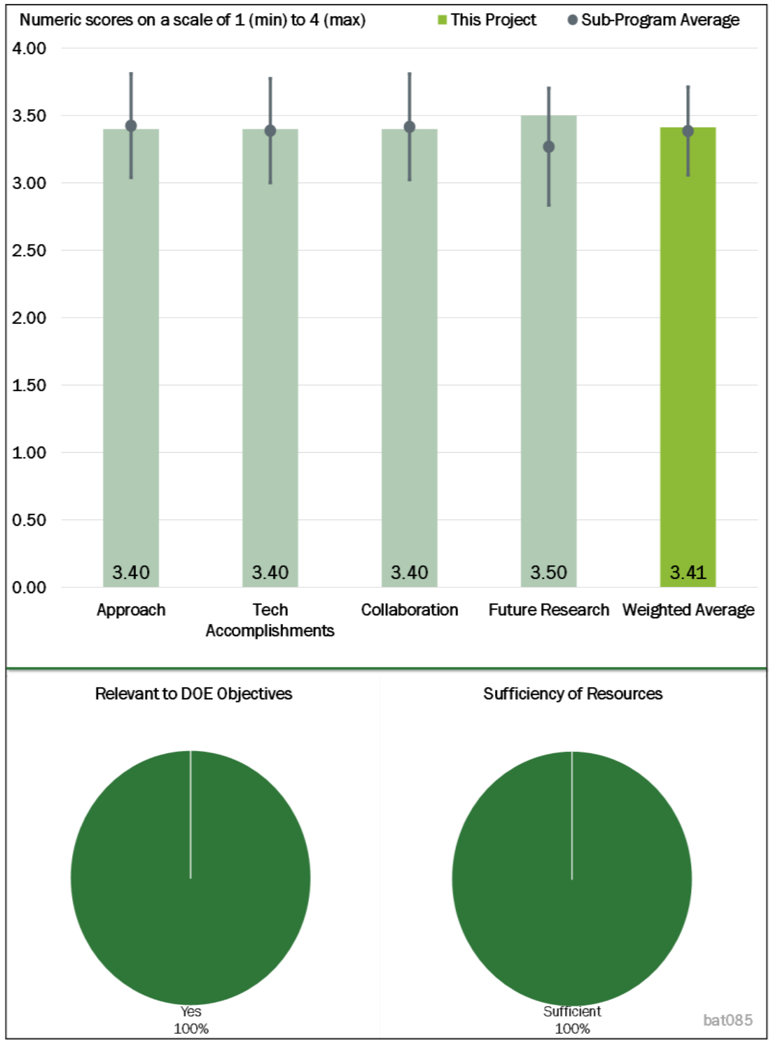

Figure 2-4 - Presentation Number: bat085 Presentation Title: Interfacial Processes—Diagnostics Principal Investigator: Robert Kostecki (Lawrence Berkeley National Laboratory)

Presenter
Robert Kostecki, Lawrence Berkeley 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 and well-planned.

Reviewer 1:
The reviewer remarked that the approach taken by the project team is focused, in-depth, and is likely to make progress in identifying the key materials degradations that are occurring and which limit the performance of a Li+ battery. The reviewer noted that using several spectroscopy and microscopy characterization techniques should greatly add to the knowledge base.

Reviewer 2:
The reviewer stated that all the analytical technologies in this program are well-designed to investigate the surface of cathode, which the reviewer finds really important to understanding the mechanism of CEI formation. The reviewer said that utilizing thin-film NMC model electrodes is a great idea to allow more techniques to be applied.

Reviewer 3:
The reviewer commented that the work is well-structured, especially the combination of the different techniques that are examining the same phenomena as a potential way to solve some of the side reaction chemistry that is occurring on the surface of Ni-based oxide active materials.

Reviewer 4:
The reviewer remarked that the objective is to develop new diagnostic techniques (e.g., both in situ and ex situ and far- and near-field optical multifunctional probes) to obtain detailed insight into electrode and electrolyte interfaces at high spatial resolutions. The reviewer noted that the project team has specifically focused on developing thin film, binder-free model cathodes using pulsed laser deposition (PLD), which are cycled in test cells, and analyzed ex situ using sophisticated characterization techniques for understanding the interfacial film-forming reactions involving electrolyte. The reviewer said that this approach allows for understanding the

interfacial changes occurring in the cathode materials from the reaction involving electrolyte or the bulk changes, including metal dissolution from the cathode. The reviewer stated that this study will have significance if extended to different high-voltage electrolytes with selected film-forming additives and also high-voltage and high capacity Ni-rich NMC cathode on the cathode with and without coatings. The reviewer said that in principle, this project is well integrated with the other projects under Applied Battery Research for Transportation (ABR) focusing on developing high-voltage electrolytes or Ni-rich cathodes. The reviewer expressed that this project would be even more beneficial if this study provides insights in designing new cathodes (and electrolytes) with improved interfacial stability.

Reviewer 5:

The reviewer said that the thin film NMC (5:3:2) was successfully made by the PLD method. The reviewer noted that the CEI layers were identified by near-field infrared (IR), attenuated total reflection (ATR)-Fourier-transformed infrared spectroscopy (FTIR) and that a mechanistic diagram was presented for the formation of CEI. The reviewer also noted that its thickness is qualitatively related to the increase of interfacial impedance. The reviewer remarked that the experimental evidences for the CEI formation are very helpful in understanding the performance of NMC in Li+ batteries. The reviewer said that it is a pity that other compositions such as 6:2:2 or 8:1:1 were not analyzed, although a reviewer suggested it in 2017.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer expressed that the project team made significant progress in providing insights into how the cathode electrolyte interphase of an NMC cathode effects cell performance.

Reviewer 2:

The reviewer remarked that good progress has been accomplished in unraveling the composition of the CEI on the NMC-532 model electrode, the non-uniform outer layer based on polyethylene glycol, and a uniform and dense inner CEI layer consisting of various Li-electrolyte species (Li alkyl carbonate [$ROCO_2Li$], Li alkoxy species [ROLi], and so on), which can contribute to the impedance towards lithiation and de-lithiation. The reviewer said it is surprising that there is no inorganic component in the inner layer involving the Li salt, as is seen on the anode. The reviewer noted that overall, the progress achieved is quite meaningful and relevant to DOE goals. The reviewer suggested that these studies extend to different electrolytes and cathodes to help with the ongoing efforts in the ABR. For example, the reviewer said it would be easier to assess different electrolytes with NMC-532, compared to cathodes with different compositions. The reviewer said inferences from this study will need to be integrated with findings from similar surface characterization studies under ABR to have a more cohesive and complete picture of the CEI.

Reviewer 3:

The reviewer commented that a lot of good work has been done in the past year. The reviewer would still like to see more data related to Ni-rich materials instead of only NMC-532. The reviewer said because the Umicore is a program partner, it should be relatively easy to conduct some tests by using their Ni-rich materials such as NMC-622 or even NMC-811.

Reviewer 4:

The reviewer said the project team presented results that clearly indicate the relation between surface chemistry and side reactions. The reviewer commented that the information obtained in the project can be helpful in designing new materials and stabilization efforts of existing materials. The reviewer suggested that a more comprehensive study looking at different Ni and Co contents in the cell could decipher side effects of increasing energy content in the material and further provide insight on the surface stabilization of the different materials.

Reviewer 5:

The reviewer commented that the CEI formation was qualitatively observed and its thickness is found to be directly proportional to the increase of impedance. The reviewer remarked that if such a relationship can be quantified by artificially adding the major components of CEI, it would be nicer.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the group at LBNL has an excellent collaboration in the national laboratory network and additionally has interactions with universities and two companies. The reviewer noted the input of the two companies mentioned is unclear.

Reviewer 2:

The reviewer said that close collaboration with national laboratories, universities, and industry was evident in the preparation of the thin film sample and the characterization methods development.

Reviewer 3:

The reviewer remarked that collaboration looks strong and sufficient. The reviewer noted that the team did not explicitly explain the role of academic and industry partners.

Reviewer 4:

The reviewer observed significant collaboration with the national laboratories, academia, and industry. The reviewer said it was unclear how each collaborator was contributing to the effort.

Reviewer 5:

The reviewer noted that there are good collaborations with several researchers at LBNL and at other DOE laboratories. The reviewer said it would be have been helpful to list the specific activities in which each of the collaborators is involved. The reviewer expressed that that collaboration with researchers developing new high-voltage electrolytes and high-capacity cathodes would be more beneficial.

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

Reviewer 1:

The reviewer stated that the proposed future work includes objectives to investigate state-of-the-art material (i.e., Ni-rich and NMC materials) and the interaction of the active material with inactive components in the electrode. The reviewer commented that these are both topics of high importance and are relevant not only for academia, but also to the Li-cell application itself. The reviewer suggested the project team look at the dynamic interaction of the different components in the composite electrode because this could potentially identify the so-far unknown side reactions, which in turn could be critical for the thermodynamic stability of the system.

Reviewer 2:

The reviewer said the proposed future work is important and logically should be completed in order for a comprehensive understanding of the interfacial properties between electrolyte and NMC cathodes. The reviewer stated that quantification is the key word for the next year of research.

Reviewer 3:

The reviewer noted the proposed future research is good and adequate to cover the next year.

Reviewer 4:
The reviewer remarked the proposed future studies seem to be well organized. The reviewer observed these studies are directed to Ni-rich NMC model systems of different compositions to understand the impedance distribution at each interface, and to quantify the effect of each of the side reactions manifesting in surface films of varying impedance at the cathode electrolyte interface during cycling. The reviewer commented that working closely with the other project teams will undoubtedly be useful to utilize this fundamental understanding in the development of electrolyte and electrodes with stable interfacial properties.

Reviewer 5:
The reviewer said future efforts to work with Advanced Battery Materials Research and industry partners to establish clear connections between diagnostics, theory and modeling, and cell developments are important.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
This reviewer said the project supports the DOE objectives really well. The reviewer noted that understanding the surface layers on the cathode is vital for the development of the high-energy Li+ battery.

Reviewer 2:
The reviewer responded yes, this project does support overall DOE objectives. The reviewer said to enable high-energy materials in Li-ion cells, it is crucial to understand the degradation mechanism occurring on the surface of the material.

Reviewer 3:
The reviewer said this effort is attempting to understand the degradation mechanism of cathode materials for EVs and this clearly supports DOE objectives.

Reviewer 4:
The reviewer observed the project is focused on developing advanced characterization techniques to understand the bulk and interfacial properties of the electrode materials in correlation with their electrochemical behavior. The reviewer also noted the project is integrated with the efforts from other groups in the ABR program. The reviewer commented that performance loss in a Li+ cell during cycling is attributed to the impedance growth, either from the organic layer formed from the reactions with the electrolyte, or the inorganic layer from the surface reconstruction resulting from metal dissolution. The reviewer noted that for designing stable electrodes in conjunction with the high-voltage electrolytes, it is essential to understand these interfacial processes, as the project team has done here. The reviewer remarked that for a widespread use of EVs and PHEVs, batteries with higher energy and lower cost than the current Li-ion batteries are needed. The reviewer said that high-voltage and high-capacity cathodes in conjunction with new high-voltage electrolytes are expected to boost the specific energy and also lower the cost of low-Co formulations, and this is consistent with the goals of the DOE VTO.

Reviewer 5:
The reviewer remarked that interfacial properties play a key role in the stability and safety of Li+ batteries by determining the capacity retention as well as the thermal properties derived from internal resistance.

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 the resources are adequate for the scope of the project.

Reviewer 2:
The reviewer believed the team has enough resources to achieve their project goals.

Reviewer 3:

The reviewer commented that the current resources are sufficient to achieve the project targets.

Reviewer 4:

The reviewer stated the resources appear to be adequate for the effort undertaken.

Reviewer 5:

The reviewer remarked that $440,000 a year seems more than enough for 0.3 full-time equivalent and one postdoctoral researcher, but there might be overhead charges or other costs that are not shown in detail. As a foreign reviewer, this was not questioned.

Presentation Number: bat106
Presentation Title: High-Capacity, Multi-Lithium Oxide Cathodes and Oxygen Stability
Principal Investigator: Jagit Nanda (Oak Ridge National Laboratory)

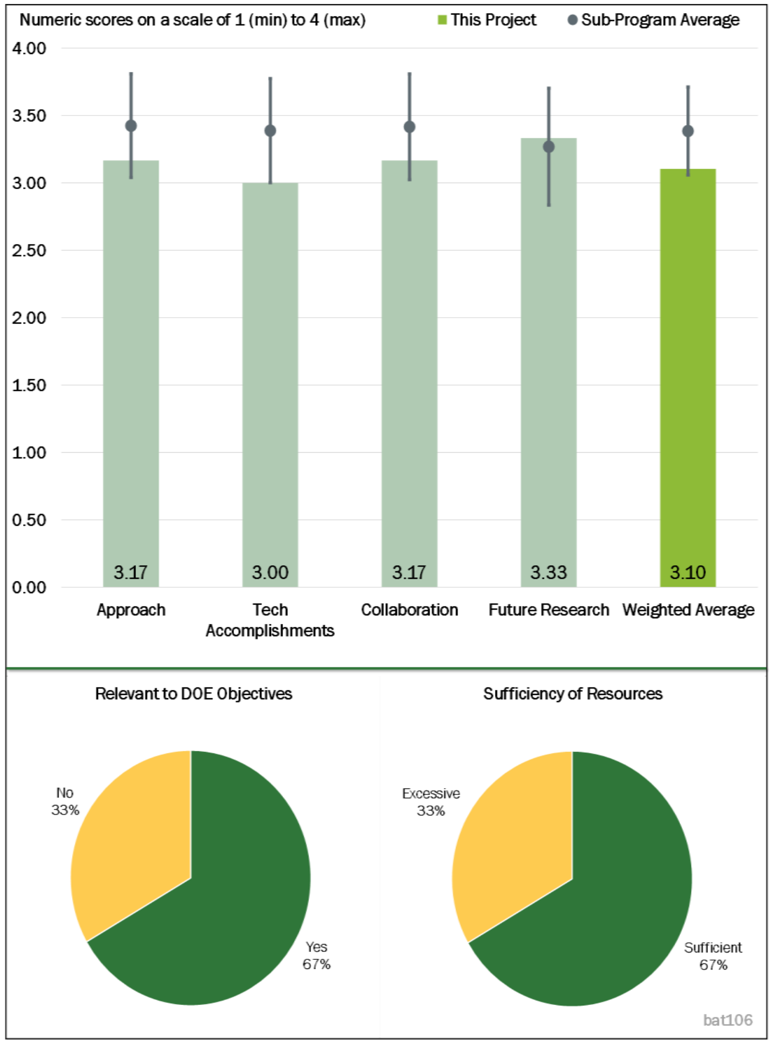

Figure 2-5 - Presentation Number: bat106 Presentation Title: High-Capacity, Multi-Lithium Oxide Cathodes and Oxygen Stability Principal Investigator: Jagit Nanda (Oak Ridge National Laboratory)

Presenter

Jagit 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 and well-planned.

Reviewer 1:

The reviewer said high-Ni-NMCs have been demonstrated as high-energy density cathode materials for next-generation Li+ batteries but the fast capacity fading has been one of the key barriers to commercialize those electrode materials. The reviewer commented the project team applied Li_2MoO_3 as structural unit for stabilizing the NMC material, which is a novel approach.

Reviewer 2:

This reviewer remarked that the project synthesizes an in-depth analysis of Li-excess and multi-Li chemistries for high voltage, high capacity cathodes. The reviewer said the project team made model driven synthetic approaches including solution-based, colloidal solution-integrated network (sol-gel), and solid-state methods. The reviewer noted diagnostic tools include a suite of microscopic, spectroscopic, and analytical techniques.

Reviewer 3:

The reviewer commented the technical aspects of the work appear to be performed reliably and with care. The reviewer cautioned that the relevance of this work is questionable when compared with the stated goals of Battery 500 (i.e., 500 Wh/kg for 1,000 cycles) and the project's specific objectives. The reviewer remarked the selection of Li_2MoO_3 appears to be a poor choice because of a 1 Li-reversible theoretical energy density (170 mAh/g) that is already lower than current state-of-the-art high-Ni NMCs 622 and 811. Furthermore, the cost of molybdenum (Mo) is not an insignificant factor when compared with Ni and Mn, and assuming a low percentage of Co in the next-generation cathode chemistries. The reviewer said that although oxygen reduction–oxidation may be a viable pathway to achieve higher capacities, Slide 7 indicates that only 1 Li is reversibly intercalated up to 4.8V and oxygen redox does not participate in the reversible chemistry. The reviewer explained that degradation due to oxygen gassing above this potential would be a safety concern and would be very negative for cycle life, but this is not the main drawback of this material. The reviewer noted that findings from the past year confirm several reports dating back at least to 2014 that show Li_2MoO_3 exhibits poor reversibility, but offer little additional insight. The reviewer said that although the true purpose of this project may be to stabilize layered NMC materials, this aspect of the effort seems poorly designed. The reviewer expressed that cycling results involving the Mo-NMC composite cathodes show that there is no apparent benefit to mixing these two cathode compounds. The reviewer said the selection of NMC-111 is unfortunate since NMC-111 is already relatively stable and does not represent the highest capacity state-of-the-art material. The reviewer concluded, it is therefore unsurprising that the project findings show poorer cycle life and capacity behavior for the composite than NMC-111 alone, and that instead using NMC-811 would be desirable to show a benefit from the composite.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that the work presented identified chemical and structural changes that occur in Li_2MoO_3 cathodes during electrochemical cycling. The reviewer commented that the project team unraveled mechanisms of electrochemical activity and degradation of Li_2MoO_3 cathodes using a combination of X-ray and neutron diffraction, Raman spectroscopy, electrochemistry, gas evolution experiments, and TEM. The reviewer said the project team developed synthesis routes to produce composite NMC-based cathodes containing a Li_2MoO_3 structural stabilizing unit.

Reviewer 2:

The reviewer said the project team applied Li_2MoO_3 to stabilize high-Ni NMCs. The reviewer noted that although experimental results showed this approach might have potential, the limited cycle number and the lack of deep structural analysis and mechanism study did not provide solid evidence to support the claims of the project team.

Reviewer 3:

The reviewer stated progress has been made to understand the mechanism of Li_2MoO_3 degradation during cycling, namely the importance of a phase change, which is irreversible. However, there has been no improvement made to the Li_2MoO_3 material that would indicate its ability to meet the Battery 500 500 Wh/kg goal or its cycle life goal. The reviewer commented that as part of a composite, or as a representative of similar compounds, the Li_2MoO_3 results from this year appear to discourage further research into this strategy of improving cathode energy density.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noticed the work has been collaborated among several partners. However, the reviewer believed there is still a gap to understanding the structure and electrochemical mechanism of the new material, but that understanding can be achieved through the collaborative work.

Reviewer 2:

The reviewer said collaboration across the project team is apparent. The reviewer would have expected a greater volume of data from such a diverse team.

Reviewer 3:

The reviewer noted the project team works with PNNL, BNL, and LBNL.

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

Reviewer 1:
The reviewer stated the proposed future work can provide additional results that were missed in the current report. The reviewer noted that the project team should consider the timeline. The reviewer noted the project will be completed by September 2018 and therefore suggested that the planned items should be prioritized.

Reviewer 2:
The reviewer observed that the work is planned in a logical manner.

Reviewer 3:
The reviewer said that the proposed future work could be interesting from a purely research perspective; however, additional justification would be necessary understand the potential benefits of early TM substitution beyond Mo and Cr. So far, the reviewer has not seen substantial progress from this project toward the high-energy and high-cycle life goals, and the reviewer would be skeptical of a new approach based on the same group(s) of materials.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer noted that Ni-rich NMCs are key cathode materials for high-performance Li+ batteries. The reviewer stated this project investigated a novel approach to stabilize the Ni-rich NMCs.

Reviewer 2:
The reviewer commented that the project objective is to develop high-voltage and high-capacity cathode materials for Li-ion batteries to achieve the Battery 500 goal of 500 Wh/kg for 1,000 cycles. The reviewer noted recent studies have shown that specific rock salt disorder Li excess oxides enable high-voltage stability.

Reviewer 3:
This reviewer remarked that the project could in theory support DOE objectives toward higher cycle life of cathode materials. The reviewer remarked that the way the research was designed and executed makes the output somewhat irrelevant to performance 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 the resources, especially the technical equipment, are sufficient to support the investigation.

Reviewer 2:
The reviewer noted that the project has achieved four out of six milestones and the rest are in progress.

Reviewer 3:
The reviewer stated that compared to highly effective projects with a similar budget, the outcomes of this project suggest that this effort may not be the most efficient use of resources.

Presentation Number: bat164
Presentation Title: Thick, Low-Cost, High-Power Lithium-Ion Electrodes via Aqueous Processing
Principal Investigator: Jianlin Li (Oak Ridge National Laboratory)

Presenter

Jianlin Li, Oak Ridge National Laboratory

Reviewer Sample Size

A total of two reviewers evaluated this project.

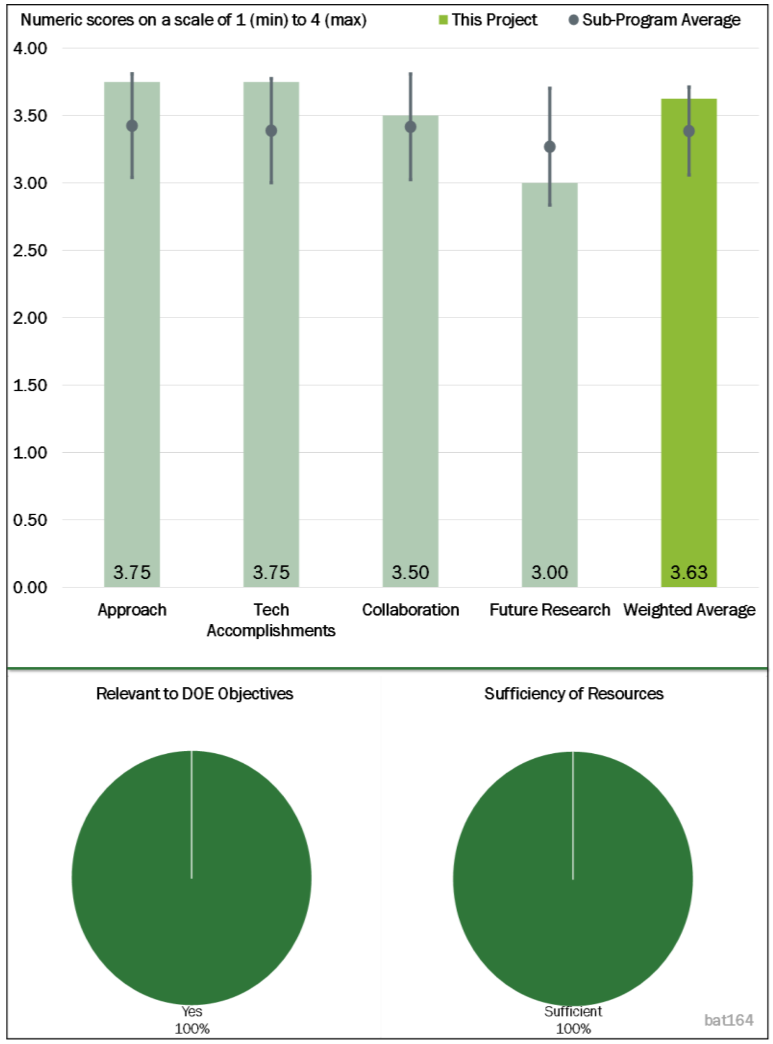

Figure 2-6 - Presentation Number: bat164 Presentation Title: Thick, Low-Cost, High-Power Lithium-Ion Electrodes via Aqueous Processing Principal Investigator: Jianlin Li (Oak Ridge National Laboratory)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer commented that using a single- and duel-sided caster system, and available aqueous binder systems, enables accelerated materials development.

Reviewer 2:

The reviewer remarked that the technical approach addressed the energy and power density and battery production cost by developing a thick electrode via aqueous processing.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said the technical approach sounds productive. The reviewer noted the progress is aligned with the plan.

Reviewer 2:

The reviewer said the team has demonstrated a successful fabrication of multilayer structure which is functional for application.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented a strong team has been put together, and noted the project team consists of academia and industry partners collaborating to attack the technical barriers.

Reviewer 2:

The reviewer pointed out that the project team has interacted and partnered with multiple national laboratories and industrial partners.

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

Reviewer 1:

The reviewer noted that the project team has an acceptable future work plan, and suggested the work plan could be improved with the addition of a specific set of metrics for the team to achieve.

Reviewer 2:

The reviewer commented that battery energy density appears to be more important than energy density for vehicle applications due to limited packing space. The reviewer suggested that the project team show the energy density of the cell with the new manufacturing processing compared to that of the base cell. The reviewer expressed that if possible, the cell level cost reduction with the new manufacturing processing should be quantized.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer remarked the project supports the goals for battery cost reduction and specific energy density increase.

Reviewer 2:

The reviewer noted that energy storage is of greater importance in the overall landscape of energy generation, use, and so on.

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

Reviewer 1:

The reviewer commented that the resources appear to be sufficient for the proposed efforts.

Reviewer 2:

The reviewer said the team has access to equipment, materials, and a technical team to sufficiently perform the described work plan.

Presentation Number: bat168
Presentation Title: Process Development and Scale-Up of Critical Battery Materials—Continuous Flow-Produced Materials
Principal Investigator: Krzysztof Pupek (Argonne National Laboratory)

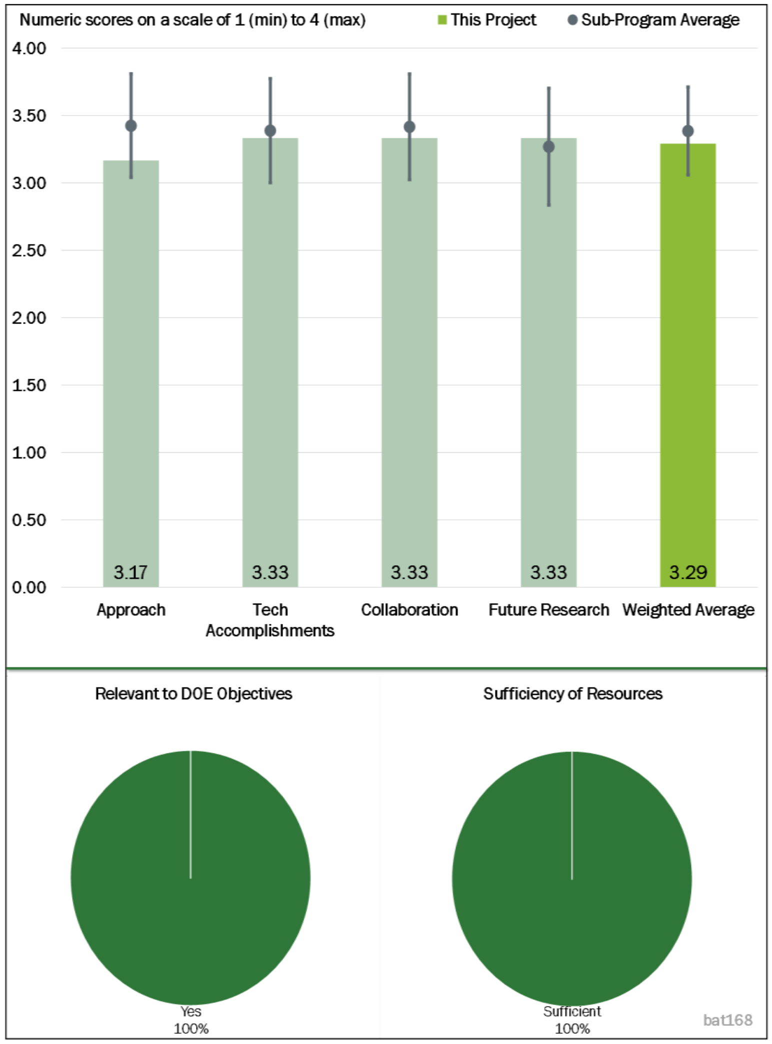

Figure 2-7 - Presentation Number: bat168 Presentation Title: Process Development and Scale-Up of Critical Battery Materials—Continuous Flow-Produced Materials Principal Investigator: Krzysztof Pupek (Argonne National Laboratory)

Presenter

Krzysztof Pupek, 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 and well-planned.

Reviewer 1:

The reviewer said the project team collected information about new materials and evaluated new, emerging manufacturing technologies to design the continuous flow reactor-based reaction to realize scale-up synthesis. The reviewer said that this is an excellent and effective approach to perform the work.

Reviewer 2:

The reviewer remarked that having a reliable source of high interest materials for development and characterization is an important aspect of material evaluation in battery systems. The reviewer said this work attempts to use certain “high volume” lab techniques to determine if some materials can be produced in a repeatable, reliable manner. The reviewer said that it is presumed that if materials are amenable to this approach at this scale, then materials may also be amenable to continuous processing at a commercial scale, although this is not a given.

Reviewer 3:

The reviewer remarked the project approach is fairly solid, with a focus on scale-up from “beaker to jug.” The reviewer acknowledged the emphasis on continuous reactors and green chemistry is appropriate to start bridging bench scale with industrial scale. The reviewer elaborated on several doubts about this approach. First, the reviewer noted the scale being attempted, which the presentation stated is on the order of 500 g or possibly up to the kilogram scale. The reviewer said while this constitutes a scale-up for sampling, it does not begin to approach a pilot scale that would be needed for truly bridging industrial production. Second, the presentation repeatedly mentioned the importance of cost in scale-up, yet this aspect of the project has been neglected. The reviewer said cost estimations for both the raw materials and processes for each compound should be considered essential to this work and perhaps could help in the downselection of compounds to be synthesized. Third, the decision-making process for which compounds to produce is selected is fairly opaque. The reviewer noted that there was some discussion during the presentation about a program manager review at the start of each scale-up, but what goes into this review is unknown. The reviewer would like more information about if these compounds are exclusively developed at national laboratories or requested by an industry partner, or if there is a known barrier to scale-up that this effort can address. Fourth, there is not enough feedback from the partners that sample these materials. The reviewer said in order to gauge the value of this effort we would have to know whether the materials being supplied are of industrial use and whether they enable a performance benefit. The reviewer noted part of the material sampling process should involve some requirement that evaluation data be shared. Fifth, in order to understand the benefit of the scale-up effort, more details about the quality of the material being produced and whether this is better or worse than the bench scale processes are needed. The reviewer said impurity concentrations and reactant utilization are standard metrics for success in such an effort.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer pointed out that the key project accomplishments are developing a cost-effective process to synthesize the advanced battery materials. The reviewer remarked that the team has successfully developed several novel electrolyte additives in the targeted timeline.

Reviewer 2:

The reviewer stated that some of the materials were amenable to this approach and that some were not. The reviewer said that this is perhaps not unexpected. The reviewer commented that it would have been helpful to provide an update on how much material of each type was produced and how many samples have been delivered for evaluation.

Reviewer 3:

The reviewer remarked that the synthetic accomplishments of this project are admirable. The reviewer commented that several Si containing solvents, fluorinated additives, and Li salts have been produced in continuous processes at scales of hundreds of grams and sampled to partners. The reviewer said that although the approach to solid-state electrolytes (SSEs) was unsuccessful, this finding is not much of a surprise. The reviewer reiterated that, as stated previously, the effort to scale-up itself should be justified by the end result of the partners who sample the material and therefore, more data on how these materials are used is necessary going forward. The reviewer said that the cycling data presented for Si containing carbonate electrolytes is an insufficient justification, because the value of this material is as a flame retardant. As the PIs are no doubt aware, reviewers also require more information about the particular test conditions for each electrochemical cell because the compatibility of solvents, additives, and salts depend on the electrode materials used.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that this project has linked with many research institutes and companies, and has been intensively collaborated.

Reviewer 2:

The reviewer commented that collaboration between Materials Engineering Research Facility (MERF) and research scientists within ANL appears to be effective. The reviewer noted that it will be important, however, to strengthen the collaborations between MERF and outside partners who sample materials in order to obtain feedback and results that guide future scale-up development and research.

Reviewer 3:

The reviewer stated that the collaboration appears to be sufficient. It is critical that the choice of materials for development as well as the ability to distribute it to a wide audience be highly collaborative. Per the reviewer, the effectiveness of this project depends entirely on serving the community's needs.

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 remarked that the main target of this project is continuously developing a scale-up synthesis approach. The reviewer reported that optimization and evaluation of new materials has also been planned.

Reviewer 2:

The reviewer indicated that the activities for the next FY are largely a continuation of existing efforts and new materials will be identified and scaled. However, the reviewer recommended that the number of materials to be scaled is reduced, to allow complementary efforts including greater emphasis on cost analysis, innovation in scale-up processes to address industry shortcomings, and verify the usefulness of the materials being produced.

Reviewer 3:

The reviewer had no special comments on future directions.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer stated that the project is a key missing link between inventing new advanced battery materials, performing a market evaluation of these materials, and manufacturing at high-volume, reducing the risk associated with the commercialization of new battery materials.

Reviewer 2:

The reviewer commented that the materials research on promising materials candidates cannot occur without a consistent, viable source of the target material.

Reviewer 3:

The reviewer stated that this effort supports DOE objectives to transfer R&D materials into industry. The reviewer said that sampling larger scales of materials is important, but it must be complemented by better engagement and feedback from industry partners.

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

Reviewer 1:

The reviewer remarked that the resources appear sufficient, but additional resources may help to expand the scope and synergistic activates (as previously described) that will make this effort even more valuable.

Reviewer 2:

The reviewer stated that the resources, including both collaborative support and in-house capability, are sufficient to perform the research activities for this project.

Reviewer 3:

The reviewer had no comments on resources.

Presentation Number: bat183
Presentation Title: In Situ Solvo-Thermal Synthesis of Novel High-Capacity Cathodes
Principal Investigator: Feng Wang (Brookhaven National Laboratory)

Presenter

Feng Wang, Brookhaven National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

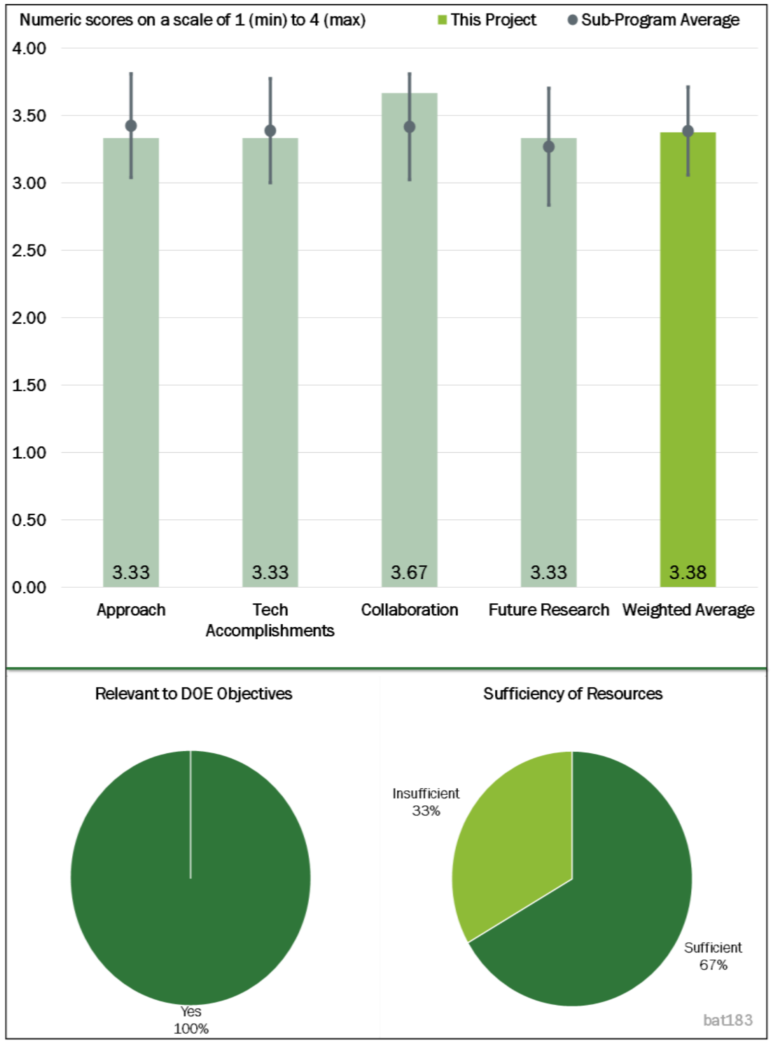

Figure 2-8 - Presentation Number: bat183 Presentation Title: In Situ Solvo-Thermal Synthesis of Novel High-Capacity Cathodes Principal Investigator: Feng Wang (Brookhaven National Laboratory)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer commented that this project is well designed and focused on understanding the synthesis parameters that influence the crystal structure of high Ni NMCs. The reviewer stated that the techniques used are complementary and varied. The reviewer pointed out that particular emphasis is placed on in situ X-ray characterization, which is excellent. The reviewer noted that because the focus of this work fundamentally uses X-ray techniques, there is a concern that the measurements are primarily of bulk crystal evolution rather than surface states, despite the use of spatially resolved spectro-imaging. The reviewer said that if future work is to focus on gradient cathodes or potential coated cathode materials, which is an area of practical concern for NMC-811, that some study of surface states would be complementary.

Reviewer 2:

The reviewer said that electrochemical performance of electrodes is highly dependent on the structural information (e.g., phase, purity, morphology, and so on) of electrode materials. The reviewer commented that this project developed the in-situ techniques to track the structural evolution of electrode materials, which will be critical to optimize the synthesis process.

Reviewer 3:

The reviewer remarked that in situ techniques are developed for structure-tracking aided synthetic design of electrode materials with desired phases and properties. However, there is a big technical challenge. The reviewer elaborated that there is no theory or design principles on synthesizing materials of desired structure and properties, and therefore the project team knows what is wanted but it is unknown how to make what is wanted.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that the accomplishments of this project provide great insights to understand the structural evolution of electrode materials from local and long range of transition metals (TMs) in NMC materials. The reviewer noted that this insightful understanding will guide the future investigation, to optimize the synthesis of high-energy density electrode materials.

Reviewer 2:

The reviewer said significant progress has been made to study the role of temperature and time on crystal structure evolution and oxidation states of TMs in NMCs. The reviewer said that the results are clear and that it will be useful in the development of high-capacity, long cycle life cathode materials. The reviewer recommended that in future work, the project would benefit from a comparison across different compositions of NMCs including NMC-622 and NMC-811, which may be more commercially relevant that NMC-71515. The reviewer noted that study of solid-state synthesis from hydroxide precursors makes sense, but that additional information on materials synthesized from carbonates or in solvothermal processes (as the project title suggests) would be equally valuable.

Reviewer 3:

The reviewer remarked that this project developed in situ techniques, allowing for multimodal characterization of solid-state synthesis under controlled atmosphere. However, designing and synthesizing specific cathode materials have proven difficult.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted the team of collaborators on this project is very strong.

Reviewer 2:

The reviewer remarked that this project is collaborated by more than 10 national laboratories and national and international universities.

Reviewer 3:

They reviewer stated that the project team works with LBNL, ORNL, ANL, Stony Brook University, Xiamen University, Alfred University, and Seoul National University.

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

Reviewer 1:

The reviewer said strong suggestions about future and ongoing work have been made to support this effort. The reviewer noted that a focus on cooling rate and Mn/Co substitution on cation ordering is a very important area of study. The reviewer said, however, more definition needs to be given to the spatially resolved techniques that could be sensitive to structural ordering. The reviewer would like to know what the recommendation is for spatial techniques and if this would this contribute to the understanding of order at or near particle surfaces.

Reviewer 2:

The reviewer believed the proposal research topics are excellent, which will focus on Ni-rich NMCs but at the same expand this technology to other batteries. The reviewer suggested linking the prepared material with the electrochemical properties, because this will close the loop of synthesis, mechanism understanding, and electrochemical properties.

Reviewer 3:

The reviewer said that the planned work includes applying the established approaches and techniques to synthesis of high-Ni layered oxide cathodes and other type of battery materials. However, given it is close to the project end date of October 2018, this could be a challenge.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer remarked that this project is very important for meeting DOE objectives toward developing higher capacity and lower Co cathode materials.

Reviewer 2:

The reviewer said the DOE overall target is to develop low-cost cathode materials with high energy density and electrochemical properties. The reviewer commented that the project focus is investigating the structural evolution of Ni-rich NMCs during synthesis, which is consistent with DOE's goals.

Reviewer 3:

The reviewer stated that the project is to develop low-cost cathode materials with high energy density and electrochemical properties (e.g., cycle life, power density, safety, and so on) that are consistent with the U.S. Advanced Battery Consortium's (USABC) 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 the resources are sufficient for this project; however, additional resources could benefit collaborative efforts and expand the scope of this very important project.

Reviewer 2:

The reviewer commented that this project has enough resources, including staff and equipment, from national laboratories and universities to achieve the goals.

Reviewer 3:

The reviewer commented that this project has achieved three out of five milestones and that one milestone has been delayed and one is pending.

Presentation Number: bat220
Presentation Title: Addressing Heterogeneity in Electrode Fabrication Processes
Principal Investigator: Dean Wheeler (Brigham Young University)

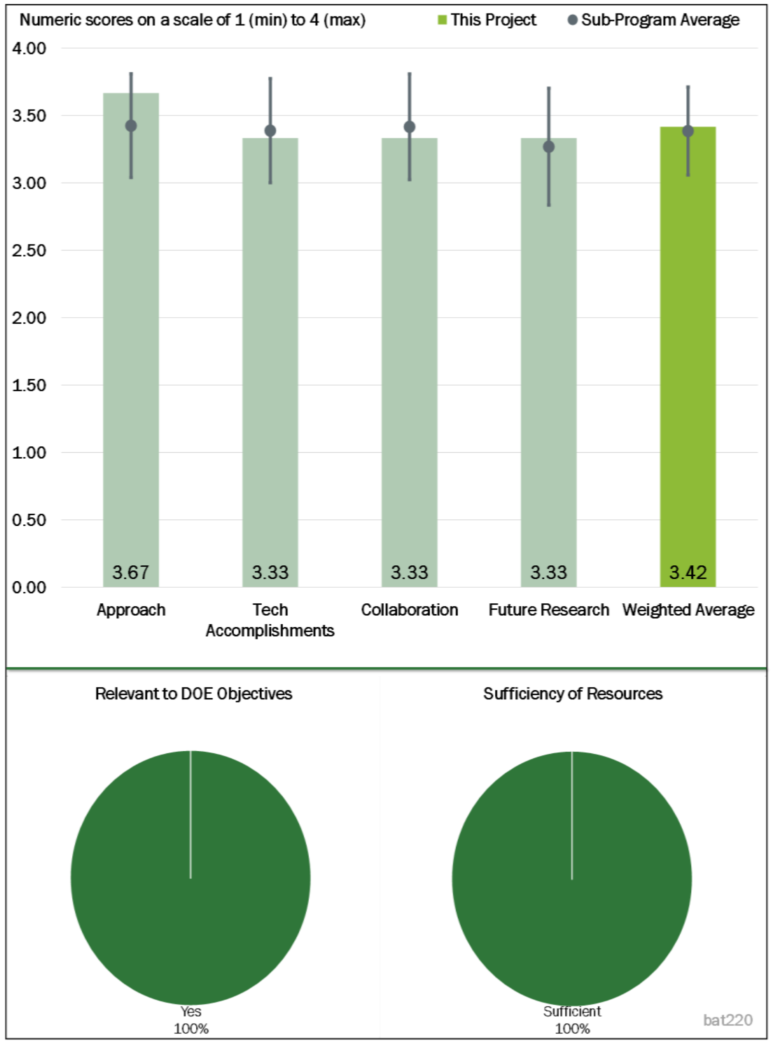

Figure 2-9 - Presentation Number: bat220 Presentation Title: Addressing Heterogeneity in Electrode Fabrication Processes Principal Investigator: Dean Wheeler (Brigham Young University)

Presenter

Brian Mazzeo, Brigham Young 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 and well-planned.

Reviewer 1:

The reviewer commented that the project team continues to do an outstanding job of developing a new technique allowing a better understanding of the effects of electrode heterogeneity of cell performance. The reviewer expressed that this effort is addressing a critical issue to the development of a long cycle-life, affordable battery.

Reviewer 2:

The reviewer remarked that the approach is outstanding and really shows a great benefit for industry.

Reviewer 3:

The reviewer noted that the device developed so far, for conductivity measurement, can reveal the situation of the electrode made from role to role. The reviewer was unable to tell how this will be applied to the fast-charged electrodes, especially after its cycling.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer expressed that the project team continues to make excellent progress. The reviewer commented that improvements were made to the micro-line probe. The reviewer explained that focused ion beam scanning electron microscopy (SEM) was used to analyze commercial electrodes and a rolling probe was developed to make conductivity measurements over large area electrodes. The reviewer said that the project team is meeting their milestones and are making significant contributions to the field.

Reviewer 2:

The reviewer remarked that a lot of great technical accomplishments have been shown in the project. The reviewer commented that the project team made a big effort to enable its technologies for industry partners and even started to sell its first commercial product. The reviewer was confused about the meaning of future technical accomplishments and was unsure if some work was ahead of schedule.

Reviewer 3:

The reviewer noted that some results were obtained for conductivity, as well as Young's modulus measurement. The reviewer remarked that there is still a significant difference between model prediction and experimental measurement for the physical properties of the porous structure. The reviewer commented that the relationship between conductivity, Young's modulus, and the fast-charging properties has not been identified.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked excellent contributions with industry (e.g., Hydro-*Québec*, Bosch, K2, and LG Chem) and the national laboratories exist.

Reviewer 2:

The reviewer stated that clearly the project team has a large collaborative network within its university, and beyond, including national laboratories and industries.

Reviewer 3:

The reviewer remarked that some improvements can be made for industrial collaborations. The reviewer noticed that all the materials tested in were from ANL and that more commercially relevant materials should be considered for future testing.

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

Reviewer 1:

The reviewer remarked that the proposed future activities are well thought-out. The reviewer said the proposed future research is logical and should lead to a technique that industry can use.

Reviewer 2:

The reviewer noted that the proposed future research is adequate for this project. The reviewer said that there are a lot of challenges that need to be overcome to enable this really cool technique. The reviewer also remarked that the speed for identification of the quality of different electrode materials was not clearly mentioned.

Reviewer 3:

The reviewer commented that there are six milestones to achieve in the remaining year. The reviewer said that besides the durability and reliability test of the conductivity measuring device, the remaining part of the project deals with the particle packing properties derived from drying and calendering. The reviewer commented that the project team wishes to do this using simulation rather than doing experiments. In fact, the drying conditions and drying technologies would significantly affect the porous structure of the electrode film made. The reviewer said the calendering conditions (nip thickness and pressure) would change the density significantly. The reviewer said that the project team should carefully consult the related literature in order to have applicable simulation results.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer commented that this project is definitely supporting DOE VTO objectives. The reviewer noted that the effort may lead to lowering cell cost. The reviewer said that battery manufacturers will have a better way to quality control their electrodes.

Reviewer 2:
The reviewer remarked that the project shows strong support for DOE objectives, which can definitely save the Li-ion industry a lot of costs.

Reviewer 3:
The reviewer remarked that the microstructure of the electrode film will have a significant effect on its electrical conductivity, its rate performance, or its charging rate. The reviewer remarked that fast charging is important for passenger cars. The reviewer stated that the project does not show any effort in overcoming the cost or capacity barriers.

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

Reviewer 1:
The reviewer suggested that DOE consider increasing the funding for this project. The reviewer hopes that this technique can be quickly applied by Li+ cell manufacture companies, which may demonstrate a big effect in the near future.

Reviewer 2:
The reviewer stated that the resources appear to be appropriate and that significant progress is being made.

Reviewer 3:
The reviewer remarked that no financial report was given and therefore assumed the project funding is sufficient.

Presentation Number: bat230
Presentation Title: Nanostructed Design of Sulfur Cathode for High Energy Lithium-Sulfur Batteries
Principal Investigator: Yi Cui (Stanford University)

Presenter
Yi Cui, Stanford University

Reviewer Sample Size
A total of five reviewers evaluated this project.

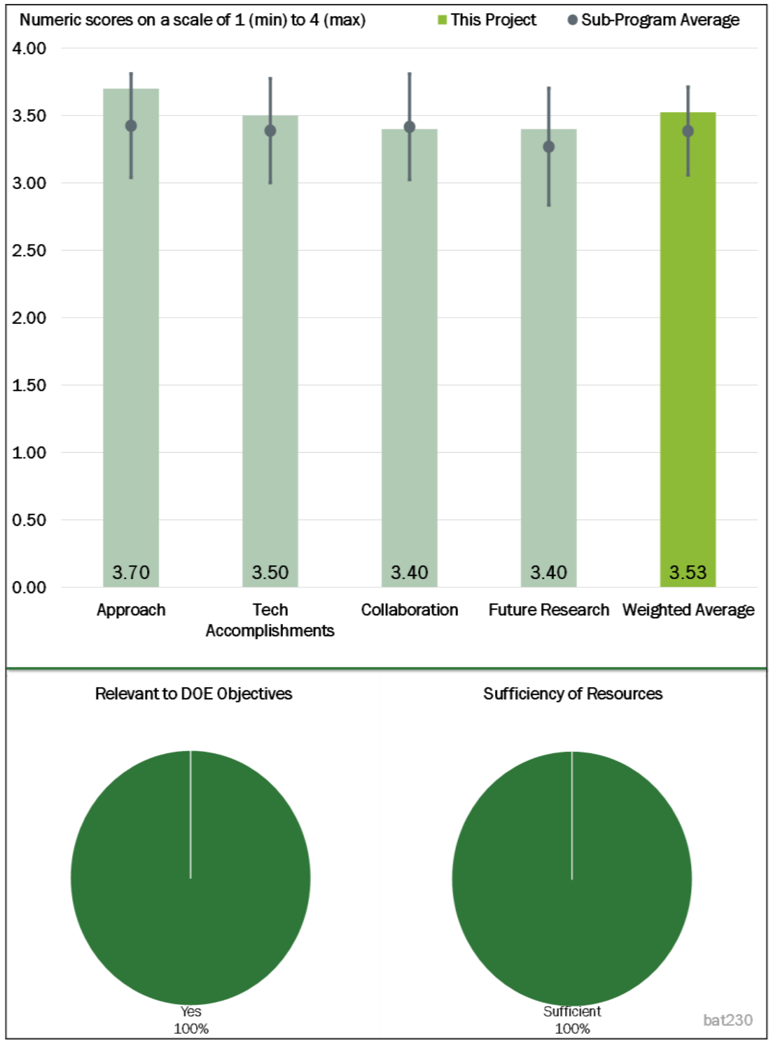

Figure 2-10 - Presentation Number: bat230 Presentation Title: Nanostructed Design of Sulfur Cathode for High Energy Lithium-Sulfur Batteries Principal Investigator: Yi Cui (Stanford University)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer remarked that based on the extensive and outstanding background research on lithium-sulfur (Li-S) from the project team, the present project made a number of new advances in this field that are of world-class quality. The findings of proper catalysts in overcoming the overpotential for Li_2S oxidation, quantifying various adsorbents for Li_2S, as well as the unique inorganic binder for Li-S cathode preparation, all represents significant achievement in their own regards. The reviewer commented that the results have been published in top ranked journals, and noted that the PI has been invited to give seminars worldwide.

Reviewer 2:
The reviewer remarked that the project team has done an excellent job in studying nanostructured design of the sulfur cathode for high-energy Li-S batteries with high capacity and stability. The reviewer commented that the project team quantitatively measured the polysulfide adsorption amount of candidate materials, uncovered different adsorption mechanisms, and identified possible adsorption species. The reviewer said that the study on multi-functional sulfur cathode binder capable of controlling of the polysulfide shuttling and facilitating Li^+ transport is of great interest. The reviewer praised the project team for making remarkable progresses in addressing the technical barriers.

Reviewer 3:
The reviewer praised the project team for an excellent approach. The reviewer commented that the project team can always find a right direction to work in and is very productive.

Reviewer 4:

The reviewer remarked that the engineering advanced nanostructured sulfur cathodes, characterization, and cell testing approach is comprehensive, focused, rigorous, and feasible. The reviewer noted that this past year the project team focused on combining theoretical calculations and experiments to identify the key parameters in determining the energy barrier for Li_2S oxidation and polysulfide. The reviewer commented that this work is definitely addressing the key technical barriers of the Li-S system.

Reviewer 5:

The reviewer summarized that objective is to develop high capacity and long-life sulfur cathode using nanostructured sulfur cathodes with: various mesoporous C hosts with and conductive polymer coating; yolk-shell with titanium dioxide-sulfur (TiO_2-S) nanoparticles; transition metal sulfide coatings; and new inorganic binders. The reviewer stated that the approach is multifaceted with several material modifications and that some of them look promising, but overall it appears to be difficult to have a quantitative comparison of the benefits from one approach to another. The reviewer remarked that the path towards maturation of one or two of these approaches is required for this development to go forward and is not detailed here. The reviewer said there was no discussion on how the Li anode will be modified to be dendrite-free and tolerant to polysulfide poisoning during extended cycling. The reviewer commented that cell designs with dense cathodes and limited electrolyte will need to be employed to demonstrate the benefits of nanostructured sulfur cathodes. The reviewer noted that the project is well integrated with the projects under Battery 500, especially with PNNL where a long-life Li anode is being developed. The reviewer noted that integrating the sulfur cathode with this anode may be beneficial later on, provided the electrolytes are compatible.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer expressed that the project team has made excellent progress this year. The reviewer commented that significant advancements were made with respect to reducing the dissolution of Li polysulfides. The reviewer noted a series of metal sulfides were investigated as polar hosts and the key parameters to polysulfide absorption were identified.

Reviewer 2:

The reviewer remarked that a number of new achievements have been obtained in addition to the vast and excellent previous results reported from the project team. The reviewer stated they are of first-class quality.

Reviewer 3:

The reviewer commented that the project team has demonstrated several technical accomplishments and progresses towards the overall project. The reviewer said the project is in good shape in terms of milestones.

Reviewer 4:

The reviewer commented on the impressive progress that has been accomplished in developing long-life sulfur cathodes with various modifications, including nanostructured C hosts confining sulfur, conducting polymer coatings, yolk-shell nanomaterial with TiO_2 over sulfur, coating sulfur with various metal sulfides, and finally using a new inorganic binder. The reviewer remarked that detailed studies have been made to understand the role of various metal sulfides (MS_2) in trapping polysulfides within the cathode. The reviewer noted that impressive publications have resulted from these studies. The reviewer summarized that overall, the progress achieved here is quite meaningful and relevant to the DOE goals. The reviewer also commented that it appears that some of these studies were made prior to the Battery 500 projects. Details on the electrode and cell design, such as sulfur loadings and electrolyte content, are missing in these charts. The reviewer remarked that this multi-faced approach, though justified in the academic environment (e.g., as topics for doctoral studies), does not look as cohesive here and some of the aspects may not be amenable to scale-up. The reviewer suggested to prioritize these approaches and integrate them, possibly for synergistic effects in larger cells, and possibly collaborating with industrial partners, because these types of studies will serve the Battery 500 project objectives better.

Reviewer 5:

The reviewer acknowledged that the project team performed enormous work. However, the project team should focus on the most recent progress, instead of listing all the accomplishments during this program. The reviewer hoped the project team can do a better job and give enough guidance for each accomplishment.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer expressed that collaboration looks really strong for this project. The reviewer noted that because the Li-S battery needs more focus on the fundamental understanding and development, a strong connection with academia is a must.

Reviewer 2:

The reviewer remarked that the project team has been collaborating with national laboratories and other universities. The reviewer noted that the collaboration is very productive.

Reviewer 3:

The reviewer stated that the project team has extended its collaboration network to include colleagues from Stanford University, a governmental laboratory, an industrial company, and two Chinese universities. In his new project's involvement with Consortium 500, he is collaborating with even more top researchers in the United States.

Reviewer 4:

The reviewer remarked that in the United States the team is collaborating with one company, Amprius, and other Battery Material Research (BMR) Program project teams.

Reviewer 5:

The reviewer remarked that there are good collaborations with several researchers within the Battery 500 project. The reviewer stated that Amprius was listed as the collaborator, but it was not clear what the collaboration is. The reviewer stated that it is probably appropriate to collaborate with the other DOE national laboratories outside the Battery 500 project or with an industrial partner (which may be Amprius) to make large format-pouch cells to demonstrate the benefits with these materials.

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

Reviewer 1:

The reviewer stated that rate capability, higher loading, and shuttle effect are still big challenges to the Li-S battery. The reviewer commented that the project team noticed those problems and has made good progress in the past to solve those problems. The reviewer concluded that the proposed future work seems logical and necessary.

Reviewer 2:

The reviewer commented that the proposed future work is well-planned. The reviewer said the project team will focus on several key tasks such as the interaction between sulfur species and multifunctional binders. The reviewer remarked that the proposed road map is very thoughtful and makes sense.

Reviewer 3:

The reviewer stated that the proposed future work is all on challenging topics facing the Li-S community. The reviewer expressed that achievement from even part of the listed tasks would make significant impact to Li-S R&D.

Reviewer 4:

The reviewer stated that future efforts are directed toward may of the issues confronting the development of a Li-S battery. The reviewer noted that although the details were not specifically identified on the slides, that the presenter was able to provide detailed plans upon questioning.

Reviewer 5:

The reviewer said that there are good collaborations with several researchers within the Battery 500 project. Amprius is listed as the collaborator, but what the collaboration would be was unclear. The reviewer opined that it is probably appropriate to collaborate with the other DOE national laboratories outside the Battery 500 project or an industrial partner (maybe Amprius) to make large-format pouch cells to demonstrate the benefits with these materials.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer expressed that for a widespread use of EVs and PHEVs, batteries with higher energy and lower cost than the current Li-ion batteries are needed, and Li-S system is expected to fulfill these needs because of the high capacity and low cost of sulfur. The reviewer stated that new high-capacity and long-life sulfur cathode materials are desired to meet DOE goals, which the project has been addressing.

Reviewer 2:

The reviewer remarked that developing stable and high capacity sulfur cathodes is critical for high energy Li-S batteries to power EVs, and is highly relevant to the VTO program goal. The reviewer commented that the approach using nano-architecture is innovative.

Reviewer 3:

The reviewer said that the project is highly relevant and is in direct support of VTO goals.

Reviewer 4:

The reviewer remarked that improvement of the high-energy and low-cost sulfur cathode material is critical for the development of the next generation of Li batteries. The reviewer noted that this project feeds this purpose really well.

Reviewer 5:

The reviewer commented that the Li-S is known for its low price and high energy capacity. The reviewer said that safe and stable Li-S is believed to be the next generation of power supply for EV or power tools.

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

Reviewer 1:

From the outstanding research outputs observed by this reviewer, the project team should have put in more resources than the allocated funding for this research topic. The reviewer elaborated that because there was no complaint from the project team about short funding that it is assumed to be sufficient.

Reviewer 2:

The reviewer stated that the project team has fully used the resources at Stanford University including the Stanford Linear Accelerator Center (SLAC) for in situ X-ray and with Amprius Inc. through collaboration.

Reviewer 3:
The reviewer said that the resources are adequate for the scope of the project.

Reviewer 4:
The reviewer believes the resources are sufficient for the project.

Reviewer 5:
The reviewer stated that the project team has the resources to complete the investigation in a timely manner.

Presentation Number: bat232
Presentation Title: High Energy Density Electrodes via Modifications to the Inactive Components and Processing Conditions
Principal Investigator: Vincent Battaglia (Lawrence Berkeley National Laboratory)

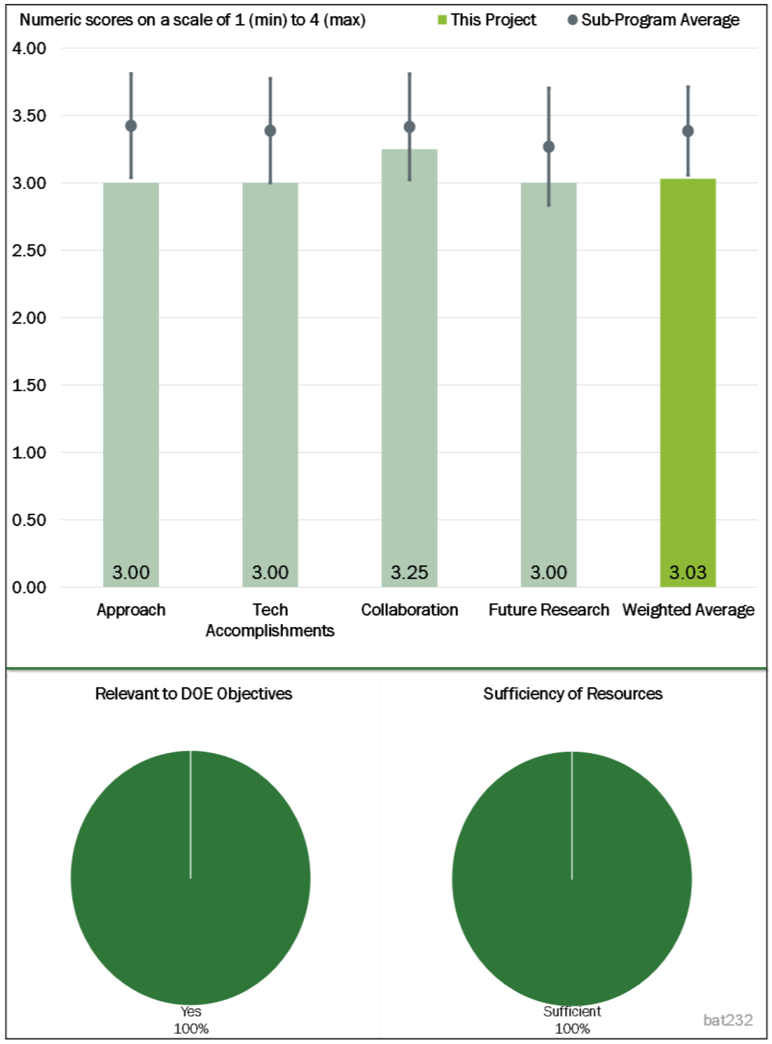

Figure 2-11 - Presentation Number: bat232 Presentation Title: High Energy Density Electrodes via Modifications to the Inactive Components and Processing Conditions Principal Investigator: Vincent Battaglia (Lawrence Berkeley National Laboratory)

Presenter

Vincent Battaglia, Lawrence Berkeley 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 and well-planned.

Reviewer 1:

The reviewer said the project team addressed the energy and power density and battery production cost.

Reviewer 2:

The reviewer stated that the approaches and evaluations of work used are standard to the industry, which is acceptable, but does not introduce anything novel to justify the project funding.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer remarked that the technical progress has been achieved as planned.

Reviewer 2:

The reviewer commented that the project team restricts itself to materials sets which preclude fabrication of thicker materials. The reviewer said the thick-film electronics industry has demonstrated capability to fabricate quality substrates of many compositions, at thicknesses of well over 1200 micrometers in thickness. The reviewer asserted that binder-solvent systems that do not “mud-crack,” yet yield thick, high-density films need to be considered.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer remarked that the collaboration across the project team members appears excellent.

Reviewer 2:
The reviewer commented that the project team has reached out to industrial partners. However, it appears the project team has not taken advantage of efforts and accomplishments at other national laboratories.

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

Reviewer 1:
The reviewer noted that the proposed work is expected.

Reviewer 2:
The reviewer was hoping to see more close talks between the project team and the battery industry for the transitioning of the technical achievement to industry, even though it was not the major focus of the project.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer remarked that the project supports the goals for battery cost reduction and specific energy density increase.

Reviewer 2:
The reviewer stated that systems with enhanced energy storage performance are desirable.

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 appear to be sufficient for the proposed efforts.

Reviewer 2:
The reviewer said the project team should take advantage of equipment and technical expertise at other national laboratories and academic institutions.

Presentation Number: bat235
Presentation Title: Characterization Studies of High-Capacity Composite Electrode Structures
Principal Investigator: Jason Croy (Argonne National Laboratory)

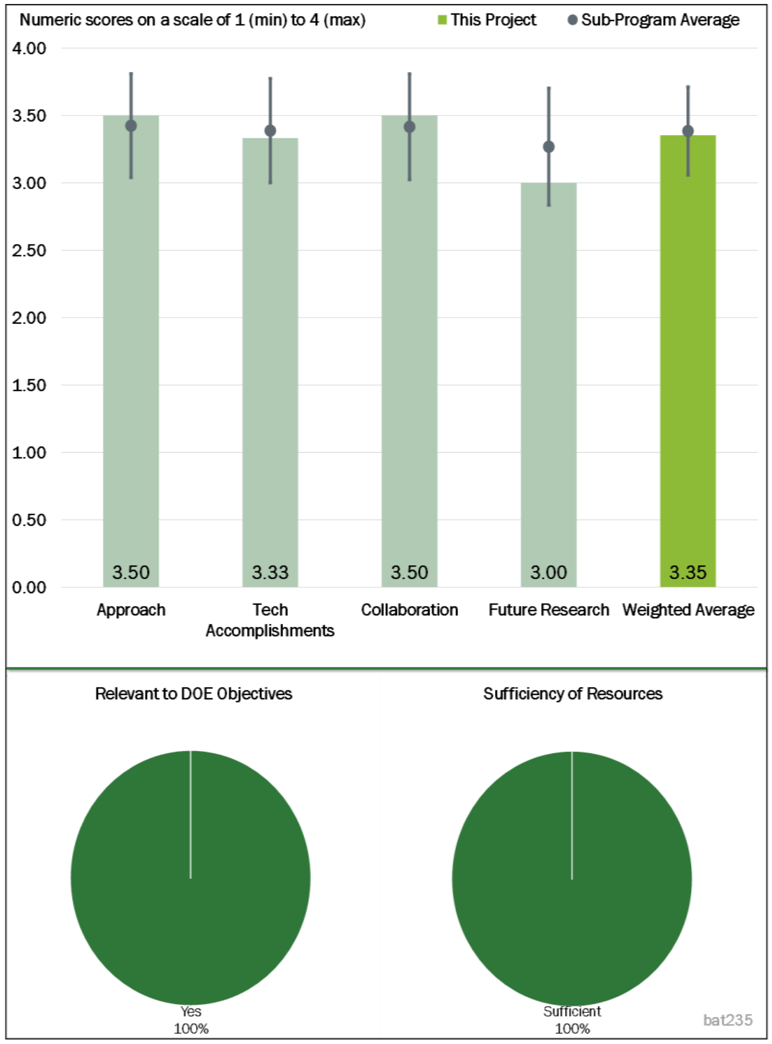

Figure 2-12 - Presentation Number: bat235 Presentation Title: Characterization Studies of High-Capacity Composite Electrode Structures Principal Investigator: Jason Croy (Argonne National Laboratory)

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 and well-planned.

Reviewer 1:

The reviewer remarked that the project approach is innovative and novel, involving the integration of spinel nano-domains directly into a high-energy LL cathode material to provide stability. The reviewer expressed that achieving reasonable dispersion of the spinel component, however, presents a synthetic challenge. The reviewer noted that cation substitution is a reasonable approach with low-temperature-lithium cobalt oxide and the decision to focus on Al substitution to achieve cycle stability was informed by prior work. Moving to a modified sol-gel approach to integrate the spinel as a composite is somewhat effective. The reviewer suggested that perhaps the most valuable effort is the thorough characterizing different compositions of LLS composites to provide a guideline for the future design of integrated spinel in LLS.

Reviewer 2:

The reviewer remarked that the project combined several resources to promise an unparalleled look into the structural, electrochemical, and chemical mechanisms in complex electrode/electrolyte systems. The reviewer commented that the work presented focused on composite LL, LLS, and endmember components in order to inform and accelerate the design of high-energy, composite cathode materials.

Reviewer 3:

The reviewer noticed that a wide array of characterization techniques including X-ray and neutron diffraction, XAS, nuclear magnetic resonance (NMR), and TEM have been applied to understand the structural information of the novel LLS high energy density cathode materials.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer remarked that the technical accomplishments and progress are excellent. The reviewer stated the project proceeds in a logical manner and many characterization techniques have been used to fully understanding the structural information of the cathode materials with various doping/synthesis approaches. The reviewer commented that all of the achievements are critical to realize the overall goals.

Reviewer 2:

The reviewer remarked that the project has made good progress toward developing strategies to improve the performance of LL cathodes. Techniques involving cation substitution and composite synthesis of LLS cathodes may be effective to achieve higher energy densities (the former likely being more reliable), although progress has been slowed by synthetic challenges. The reviewer remarked that results from the composite synthesis of LLS cathodes strategy of preparing composites by a modified sol-gel method is not convincing from an electrochemical performance perspective or the proposition of synthetic scale-up, but was obviously a risk mitigation strategy. Despite this, the thorough characterization of different composite compositions is a valuable contribution toward LLS design. Nevertheless, more effort should be placed on performance evaluation in battery cell environments, which demonstrate high energy. The reviewer remarked that using computational simulation to provide an explanation for structural damage during cycling, though interesting, could be better supported by experimental efforts.

Reviewer 3:

The reviewer remarked that the project demonstrates Al-substitution is the most effective in enhancing the cycle stability. The reviewer said synergistic performance improvement by LT Al surface treatment and electrolyte additives is confirmed in LLS//Gr full cells.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said collaboration across the technical team seems to be very effective.

Reviewer 2:

The reviewer commented that this work is a collaboration between many national laboratories (ANL and PNNL), and universities (Northwestern University, etc.).

Reviewer 3:

The reviewer noted that the project team works with different teams at ANL, the Pohang Accelerator Laboratory in Korea, PNNL, and Northwestern University.

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 project has ended.

Reviewer 2:

The reviewer noted that the project has ended.

Reviewer 3:

The reviewer remarked that the future project plan appears reasonable but that it is largely a continuation of the current strategy, which has been slowed by synthetic challenges. The reviewer suggested that perhaps a different methodology, making use of additional collaborators with experience in particle growth processes, could be utilized for faster development.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer commented that the LLS composite cathodes with suitable surface coatings are promising to provide stable structures, with high capacities at high rates and are being addressed in the project. The reviewer remarked that the project is highly relevant to the DOE goals.

Reviewer 2:

The reviewer said that this project seeks to stabilize high-energy density LLS structures, by utilizing an in situ grown spinel phase. The reviewer remarked that this effort could offer competitive cathode energy densities, but additional development is clearly needed. The reviewer commented that some effort should be recognized to reduce the use of Co and other high-cost elements in future work. The reviewer also noted that there should be some discussion of scalability of the synthesis methods if these materials are to be industrially relevant.

Reviewer 3:

The reviewer stated that cycling stability of Co-based spinel compounds is greatly improved by cation substitution, particularly with Al, and precise synthesis control approaches. The reviewer commented that full cell performances of LLS cathodes are significantly improved by surface treatment and electrolyte additives.

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

Reviewer 1:

The reviewer said the current resources appear sufficient, but there could be an opportunity to promote further collaboration with partners that have complementary synthetic experience in particle growth processes. The reviewer commented that more resources may benefit this effort.

Reviewer 2:

The reviewer noted that the resources from national laboratories and universities, including research staffs and equipment, are sufficient for the project to achieve the overall goals on time.

Reviewer 3:

The reviewer noted that the project has achieved all three milestones.

Presentation Number: bat240
Presentation Title: High-Energy Anode Material Development for Lithium-Ion Batteries, Cary Hayner, Sinode Systems
Principal Investigator: Cary Hayner (Sinode Systems)

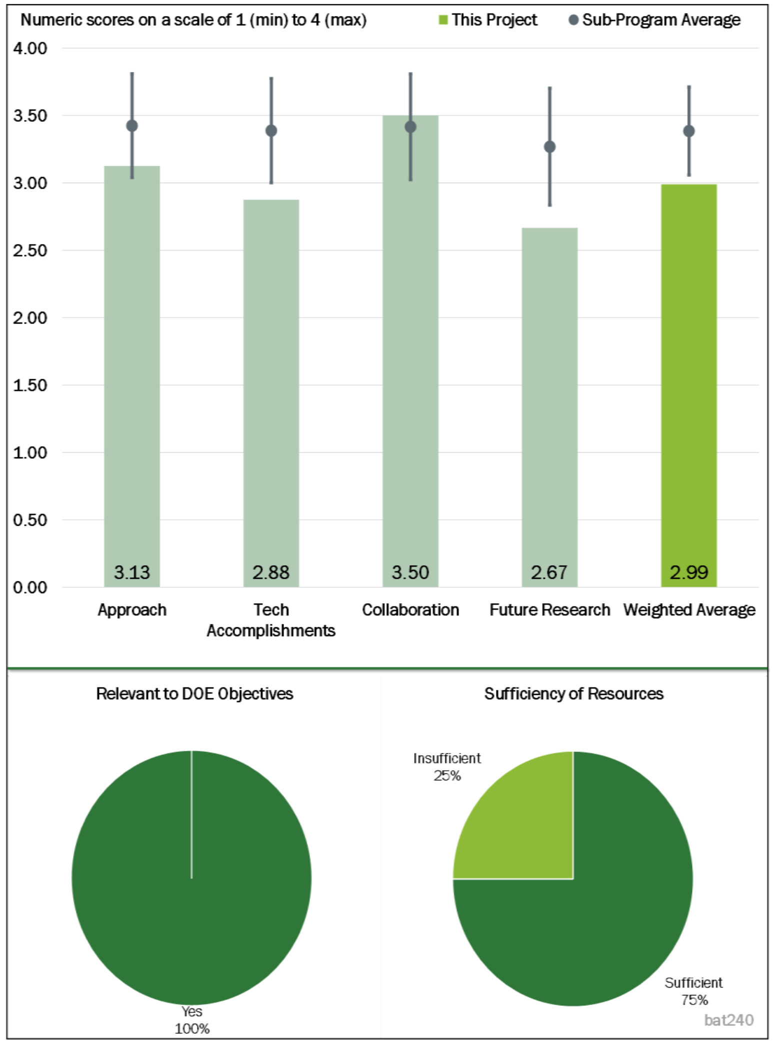

Figure 2-13 - Presentation Number: bat240 Presentation Title: High-Energy Anode Material Development for Lithium-Ion Batteries, Cary Hayner, Sinode Systems Principal Investigator: Cary Hayner (Sinode Systems)

Presenter

Cary Hayner, Sinode 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 and well-planned.

Reviewer 1:

The review explained that this is an organized project for the fabrication of the anode material, testing different formulations for the core material (Si-graphene) and adding different kinds of multilayer coatings, and selecting the best one based on cycle life and performance.

Reviewer 2:

The reviewer indicated that a good job is being done with respect to scale-up but the project is very far from demonstrating a significant chance that cycle life targets will be met.

Reviewer 3:

The reviewer would like to see Si-anode developers in general, and Si-Node in particular, address cell dimensional changes over life of cell, capacity recovery on aging and cell abuse tolerance. The reviewer said Si-Node did mention 80% capacity recovery 30 days at 60°C, which is better than nanowire structures.

Reviewer 4:

The reviewer reported that the technology is based on coating Si with graphene and optimizing the electrolyte to improve the cell. Although there seemed to be a fair amount of engineering to overcome challenges, it was not clear how transferable these solutions would be to real cells under real conditions.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer observed good progress on reducing graphene raw material cost and transition to water-base and high solid coating and that meeting cycle life has required blending the Si-anode with graphitic C. The reviewer added that progress would be easier to see if the capacity retention plots included the electrode loading and composition information.

Reviewer 2:
The reviewer commented that 1-Ah Li-ion cells have been tested and fabricated and the team is on track to fabricate 10-Ah Li-ion cells on schedule. However, cycling life of fabricated cells is less than 500, which needs to be improved to achieve commercial battery life-cycles. The reviewer added that the cycle life has been improved adding to the starting core material coating layers.

Reviewer 3:
The reviewer remarked that the project seemed to make progress to addressing performance goals though it was not clear where this technology is compared to state of the art.

Reviewer 4:
The reviewer did not see significant progress in cycle life, which is the single biggest challenge. The reviewer noted that mostly, the project showed that things do not get worse with scale-up.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted well-organized collaboration and coordination with other institutions in the fabrication process.

Reviewer 2:
The reviewer asserted that PPG and A123 are fine choices and that the project should partner with the Si deep dive to evaluate materials.

Reviewer 3:
The reviewer pointed out that SiNode has strong partners in PPG and A123 and is actively reaching out and engaging partners and potential customers. However, collaborator roles/inputs were not apparent in the presentation.

Reviewer 4:
Good partnerships were observed by this reviewer, but it was unclear how the partners are contributing or coordinating.

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

Reviewer 1:
The reviewer stated the project is near completion.

Reviewer 2:
The reviewer remarked that it is unclear how further optimization will be performed and that the cells continue to lose capacity despite changes. The reviewer questioned how the project team identifies and plans to address the losses.

Reviewer 3:
The reviewer did not get a sense that the project team has a plan for how to achieve better cycle life.

Reviewer 4:
The reviewer explained that proposed future research on material development does not show recommendations based on the acquired experience in the present work and that the recommendations are too general, such as evaluate alternative structure for significant cycle life improvement or improve active material formulation and coating/barriers to extend cycle life.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer commented the project is clearly pointing on the development of Li-ion cell with higher performance than the actual commercial ones.

Reviewer 2:
The reviewer indicated that Si anodes in principle provide significantly higher energy density.

Reviewer 3:
The reviewer highlighted Si as one of the few materials capable of reaching the energy densities required in the future.

Reviewer 4:
The reviewer noted the DOE VTO has invested significantly in Si anodes to meet EV battery cost and specific energy 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 reported that the program is 90% complete and the available resources were sufficient.

Reviewer 2:
The reviewer said the resources seem sufficient to accomplish the goals.

Reviewer 3:
The reviewer had nothing to report.

Reviewer 4:
There were no indications detected by this reviewer that the stated milestones can be met.

Presentation Number: bat241
Presentation Title: Advanced High-Performance Batteries for Electric Vehicle (EV) Applications
Principal Investigator: Ionel Stefan (Amprius)

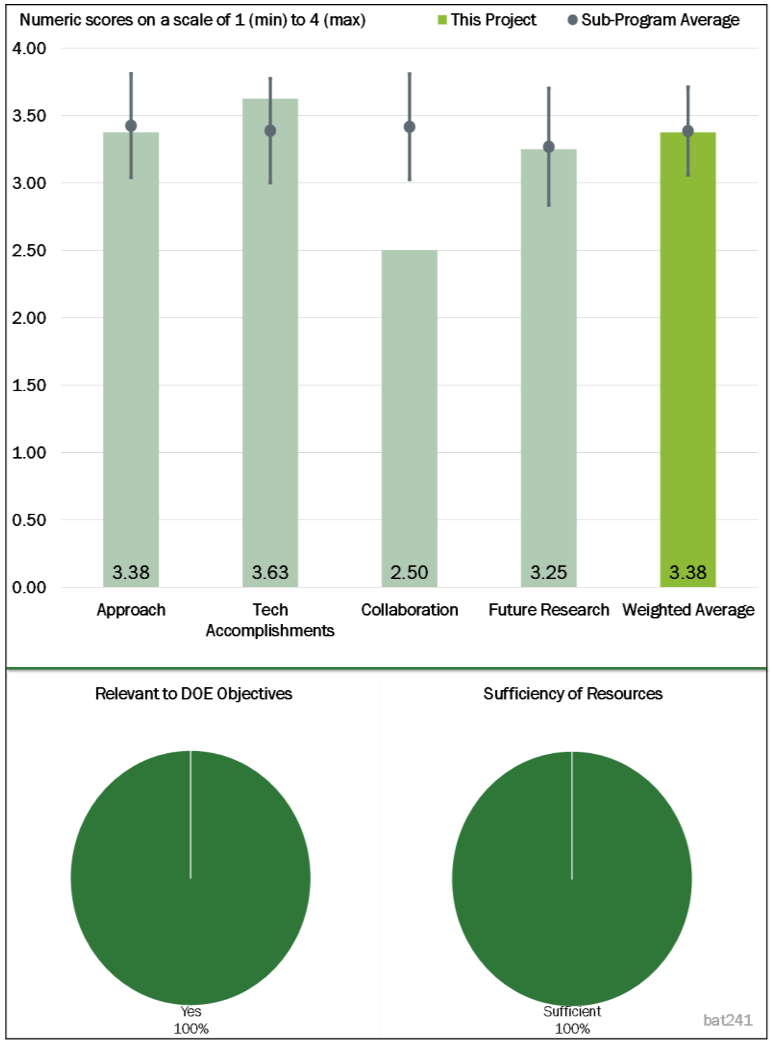

Figure 2-14 - Presentation Number: bat241 Presentation Title: Advanced High-Performance Batteries for Electric Vehicle (EV) Applications Principal Investigator: Ionel Stefan (Amprius)

Presenter

Ionel Stefan, Amprius

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 and well-planned.

Reviewer 1:

The reviewer described the strategy as a good one—the project team controls the density of the Si nanowires and their length to maximize ion transport and avoid Si-Si “collisions.”

Reviewer 2:

The reviewer indicated that the barriers were addressed effectively, and most of the objectives were reached.

Reviewer 3:

The reviewer asserted that the team has clearly made significant efforts and developing scale-up and the gassing seems to be a problem. The reviewer noted the approach to this using purely additives seems one track. The reviewer suggested the project team expand the pathways to deal with gassing and perhaps interact with DOE deep dives.

Reviewer 4:

The reviewer commented that the calendar life was identified as concern and that calendar life improvement to capacity recover was presented but needs more work. The reviewer also noted, the cell dimensional change/tolerance was not reported. The reviewer said the Amprius anode structure and porosity may be beneficial for this criterion and that progress on gas evolution was also reported but not substantiated—this is a key technical advance for high-energy prismatic pouch cells with high Ni cathode + Si anode. The reviewer noted that the principal investigator (PI) verbally noted good results in abuse testing 10 amp hour (Ah) cells at Sandia National Laboratories (SNL) and that this should be reported along with details of the cell design and test conditions. The reviewer would be interested to hear what Si % utilization is in the cell.

The reviewer pointed out that the cathode work, if any, was not really clear, and that some data seemed to be a high-voltage LCO cathode, which is a non-starter for VTO-relevant markets.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer observed considerable progress being made in all of the gap areas, and noted that performance at low temperature is not really satisfactory for any cells.

Reviewer 2:
The reviewer noted that the project is developed according to the milestones and the planned time, and that there has been important progress in increasing energy density, specific energy, and cycle life.

Reviewer 3:
The reviewer still had concerns with gassing, and noted that more focus on, and new ways to address this, is needed.

Reviewer 4:
The reviewer reported that calendar life was identified as a concern and that calendar life improvement to capacity recover was presented but needs more work. The reviewer noted that progress on gas evolution was also reported but not substantiated and that this is a key technical advance for high energy prismatic pouch cells with high-Ni cathode + Si anode. The reviewer said the PI verbally noted good results in abuse testing 10Ah cells at SNL and that this should be reported along with details of the cell design and test conditions.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer indicated that the project team has worked with several partners for the development of cathodes and electrolytes.

Reviewer 2:
The reviewer described collaboration as limited, but acknowledged that the program was single awardee.

Reviewer 3:
Although many companies were listed, this reviewer was unsure of the efforts or significance.

Reviewer 4:
The reviewed noted that the project has no partners and that this can be a fairly serious drawback because it could mean that the project team does not understand what the market is demanding. The reviewer said it can also mean that the project team is not aware of some technologies that could help advance towards the project goals. The reviewer stated the fact that the project team "work with multiple partners" does not necessarily mean very much at all.

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

Reviewer 1:
The reviewer commented that the project correctly proposed how to face the barriers in the future, and asserted that the collaboration with the other participants will be very useful to complete the project within established targets.

Reviewer 2:
The reviewer gave the project team a high score here because the project team has a good record of year-to-year improvement. However, the reviewer noted, the project team does not indicate how they will try to overcome the cycle and calendar life problems.

Reviewer 3:
The reviewer noted that the project team should think about alternative ways around the problems it is having, and that the team should maybe focus on standard cathodes to deal with only one electrode problem.

Reviewer 4:
The reviewer noted that 25% of the budget remains, but there is a 9/2018 end date and that it is not clear how the program lands on runway.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer described this project as very helpful for the DOE objectives to obtain better performance batteries that can be used in electric cars. The reviewer also noted that several promising materials are investigated in this project for the anode, cathode, and electrolyte.

Reviewer 2:
The reviewer asserted that development and demonstration of 350 Wh/kg cells and addressing gap analysis for EV application is relevant to DOE VTO objectives.

Reviewer 3:
The reviewer highlighted Si as one of the few technologies that can address future energy storage goals.

Reviewer 4:
High energy density was noted by this reviewer.

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

Reviewer 1:
The reviewer noted resources are sufficient for the development of this project, allowing that all pouch cells were delivered according to milestones.

Reviewer 2:
The reviewer found no indication that new resources are necessary.

Reviewer 3:
The reviewer stated $5 million for single company program could be challenged, but the company provided 50% cost share.

Reviewer 4:
Sufficiency of resources was described by this reviewer as self-explanatory.

Presentation Number: bat247
Presentation Title: High-Energy Lithium Batteries for Electric Vehicles
Principal Investigator: Herman Lopez (Envia Systems)

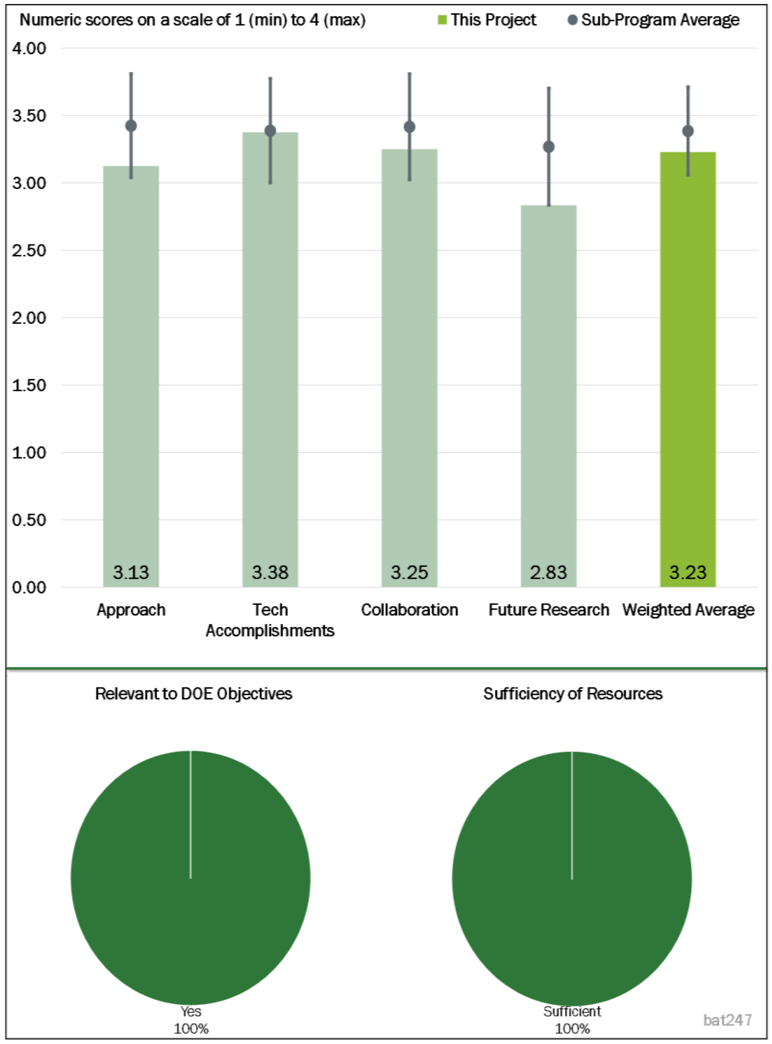

Figure 2-15 - Presentation Number: bat247 Presentation Title: High-Energy Lithium Batteries for Electric Vehicles Principal Investigator: Herman Lopez (Envia Systems)

Presenter

Herman Lopez, 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 and well-planned.

Reviewer 1:

The reviewer was very impressed with the progress this year, and would like to see calendar life measurements.

Reviewer 2:

The reviewer reported the project team aims to make incremental progress by combining their own work with the best available from collaborators.

Reviewer 3:

The reviewer explained that this project focuses on increasing the battery capacity and that other objectives, such as specific energy and life-time, are not given much effort. The reviewer also noted plots should be redone for a presentation and not simply copied/pasted from other sources because several of them are unreadable.

Reviewer 4:

The principal concern indicated by this reviewer is that this appeared to be a cathode screening exercise and the poster did not make clear what development/advances were accomplished. The reviewer noted that was an absence of even rudimentary cell chemistry or non-proprietary data on electrode design variables and the influence on performance makes this difficult to understand what work was performed.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer asserted that the project team has made outstanding progress, and the reviewer would like to see calendar life tests and elevated temperatures.

Reviewer 2:

The reviewer reported that very good results have been obtained, closing in on 300 Wh/kg and that 700 cycles is probably more than sufficient.

Reviewer 3:

The reviewer stated that some of the USABC EV cell targets for 2020 have not been accomplished yet, principally the life-time of 1,000 cycles. No results on the economical pre-lithiation process were observed by this reviewer. However, some goals such as the large capacity battery and 80% of SOC in 15 minutes have been achieved.

Reviewer 4:

Progress on cell fixturing, scale up, and gassing was reported but not translated to practicality/impact in a vehicle battery pack, which this reviewer described as an apparent significant advance in incorporating high fraction of SiO_x with unknown approach to prelithiate or manage irreversible capacity loss (ICL). The reviewer noted the fast-charge results are impressive and meaningful, but would like an explanation of how or the cycle life.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that Zenlabs has several partners and each one is specialized in building a specific part of the battery or manufacturing the cell or testing the battery. The reviewer noted the task distribution is excellent and all the partners are well-coordinate to each other.

Reviewer 2:

The reviewer observed good coordination with partners though the reviewer is not sure where pre-lithiation partner is coming in.

Reviewer 3:

The reviewer remarked that the project team seems to have organized an excellent collaboration, but the reviewer does not see what the project team is contributing, other than organizing these collaborators to all work together.

Reviewer 4:

Aside from Slide 5, it was not really clear to this reviewer what the roles were, beyond supplier.

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

Reviewer 1:

The reviewer reported that the program is ended/under a no-cost extension.

Reviewer 2:

The reviewer stated the project is mostly over and it looks like the big issue is what works best and would it apply to other systems.

Reviewer 3:

The reviewer noted this is the last year (out of 4) and all the proposed future research is completed. The reviewer also noted the project team did not propose anything new to help to overcome the barriers.

Reviewer 4:
The reviewer did not see any ideas for how to make the project team's results any better, other than downselecting from among the samples that the project team already have.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer indicated that development and demonstration of large-format, high-energy cells supports DOE objectives related to EV adoption and domestic cell production.

Reviewer 2:
The reviewer explained that the project addresses the majority of the DOE goals such as life-time, specific energy, high rate charge, and others; however, not all goals were successful but the research performed will help to accomplish the goals in the near future.

Reviewer 3:
The reviewer stated clearly this is working towards suitable approaches for high energy density.

Reviewer 4:
High energy density was noted by this reviewer.

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

Reviewer 1:
The reviewer observed reasonable resources, considering the large number of partners.

Reviewer 2:
The reviewer noted a no-cost extension was requested, but it is not clear if this indicated delays due to resource availability.

Reviewer 3:
The reviewer described resources as okay.

Reviewer 4:
Resources were fine from this reviewer's perspective.

Presentation Number: bat252
Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Electrochemistry and Evaluation
Principal Investigator: Daniel Abraham (Argonne National Laboratory)

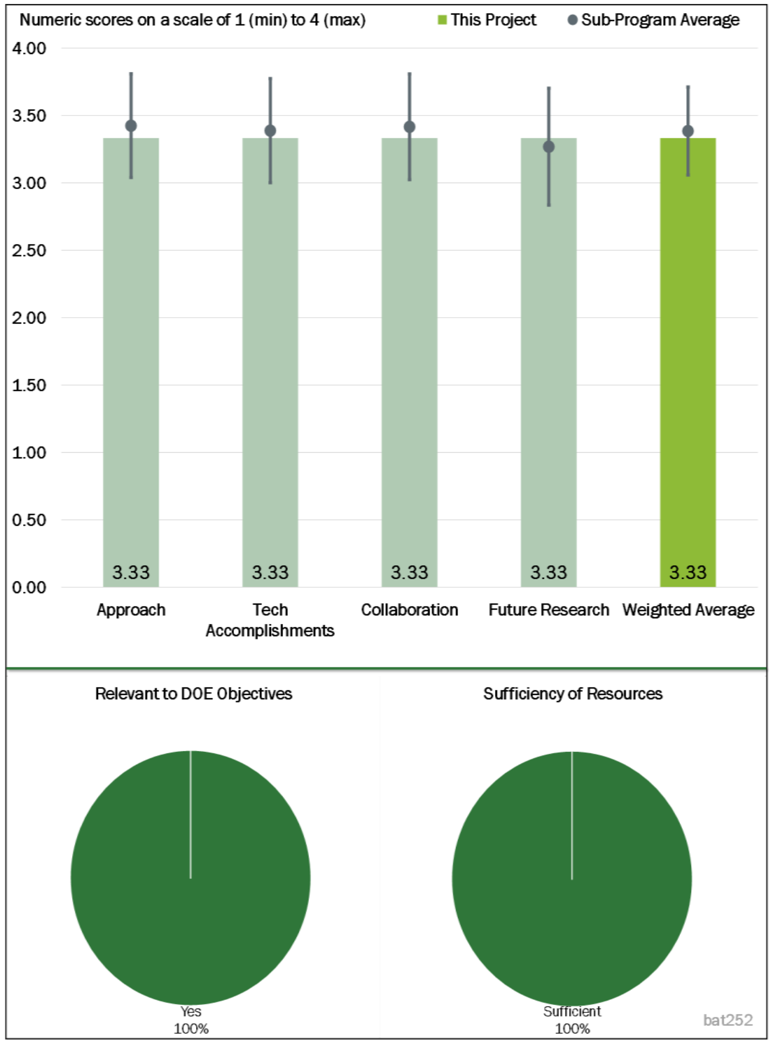

Figure 2-16 - Presentation Number: bat252 Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Electrochemistry and Evaluation Principal Investigator: Daniel Abraham (Argonne National Laboratory)

Presenter

Adam Tornheim, 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 and well-planned.

Reviewer 1:

The reviewer believed the approach taken was excellent. It proceeds in a logical manner and a wide array of characterization techniques were used to gain a better understanding of the challenges confronting the next-generation of electrode materials.

Reviewer 2:

The reviewer said this project is well-designed and supportive of modeling and materials characterization by collaborators. Generating a figure of merit for energy and power of a standard cell with different electrolytes is a critical need. The reviewer added it would be particularly desirable to share the protocol for determining these figures of merit (FOMs) with the community to standardize such evaluations. One drawback of this approach is the inherent interplay between the electrode material(s) chosen in the standard cell and the electrolyte. In essence, what might work for lithium-iron phosphate (LFP) would not be the same as LMO or Li NMC. Similarly, different graphites would exhibit different FOMs with the same electrolyte. The reviewer said the key novelty of this work is in the determination of electrolyte additive passivation mechanisms. Studies of NMC gassing at high voltages and Mn dissolution, while important, are somewhat duplicative of what is already in the published literature. The reviewer described the AEGIS system as interesting from a research standpoint, but its benefits over standard differential electrochemical mass spectrometry (DEMS) techniques remain unknown (or merely unexplained).

Reviewer 3:

The reviewer asserted that this was a very good overview of a number of separate research areas related to electrolyte interactions. The reviewer noted it was presented essentially as an overview of disparate areas of work, and could have benefited from a higher-level dialogue on the overarching theme and how these various topics may tie together as it was a little difficult to get the detail on any one topic.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that this project has made excellent strides toward aggregating understanding of electrolyte additive function. The reviewer noted that more work needs to be done in this area, but should also be accompanied by fundamental surface science studies of the sort that this project has tackled (i.e., on tris(2,2,2-trifluoroethyl) phosphite [TTFP]). The evaluation of fluorinated electrolytes is similarly important. The reviewer stated the PIs should be aware, however, of several trends in industry away from prohibited or potentially harmful compounds (i.e., sulfones, Poly[ether sulfones]).

Reviewer 2:

The reviewer explained that the project accomplishments provide great insights to understand the interfacial reactions between electrolyte and electrode materials as well as the role of electrolyte additives to the electrochemical performance of Li-ion batteries. This insightful understanding will guide the future investigation to optimize the development and synthesis of electrolyte for high-energy density batteries.

Reviewer 3:

The reviewer noted that several interesting areas of work were discussed. The observation of dramatically different behavior due to the formulation of the electrolyte in pre-formed solid electrolyte interface (SEI) layers was not necessarily a surprise, however quite interesting none the less. The reviewer noted significant follow up on this work could provide some interesting mechanistic understanding of this interesting phenomenon. Again, several topics showed interesting results, but with little cohesion between topics.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that collaboration is strong across the project team.

Reviewer 2:

The reviewer said this project was collaborated among many national laboratories and universities as shown in the presentation.

Reviewer 3:

The reviewer commented that this work was obviously accomplished with a large number of competent research components, but that it did not necessarily appear that the project team was coordinated in a strong way. This does not suggest the work was not of high quality, simply that coordination of the different components was not evident.

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:

Overall, this reviewer described the proposed future work as excellent. The reviewer suggested the PIs could pay more attention to the understanding of interface evolution, especially the interfaces of cathode/electrolyte and anode/electrolyte. Probably, techniques of high-resolution transmission electron microscopy (HRTEM) and/or soft XAS can provide more insightful information.

Reviewer 2:
The direction of the program appeared sound to this reviewer and in line with overall research goals in the field.

Reviewer 3:
The reviewer remarked that suggestions for future work are largely continuations of current efforts to understand electrolyte passivation/degradation mechanisms and the influence of gassing. This work is complementary to modeling and materials characterization efforts and so should also seek to understand the interplay of electrode coatings on electrolyte behavior. The reviewer added an improved understanding of formation mechanisms at various temperatures would be valuable. Such work was started by looking at impedance as a product of calendar aging.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer described this project as very important and extremely relevant to DOE objectives that may guide the design of electrolytes that support higher energy density battery materials.

Reviewer 2:
The reviewer stated the overall DOE target is to develop Li-ion batteries with low-cost, high energy density and electrochemical properties. This project's focus, developing high voltage electrolyte additives and understanding the reactions between electrolyte and electrode materials, is consistent with DOE's goals.

Reviewer 3:
The reviewer said that developing a modeling component of complex materials behavior is a relevant area of research.

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 sufficient resources from many national laboratories and universities to support the research work of this project.

Reviewer 2:
The reviewer described project resources as sufficient.

Reviewer 3:
The reviewer had no special comments on resources.

Presentation Number: bat253
Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Theory and Modeling
Principal Investigator: Hakim Iddir (Argonne National Laboratory)

Presenter

Hakim Iddir, Argonne National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

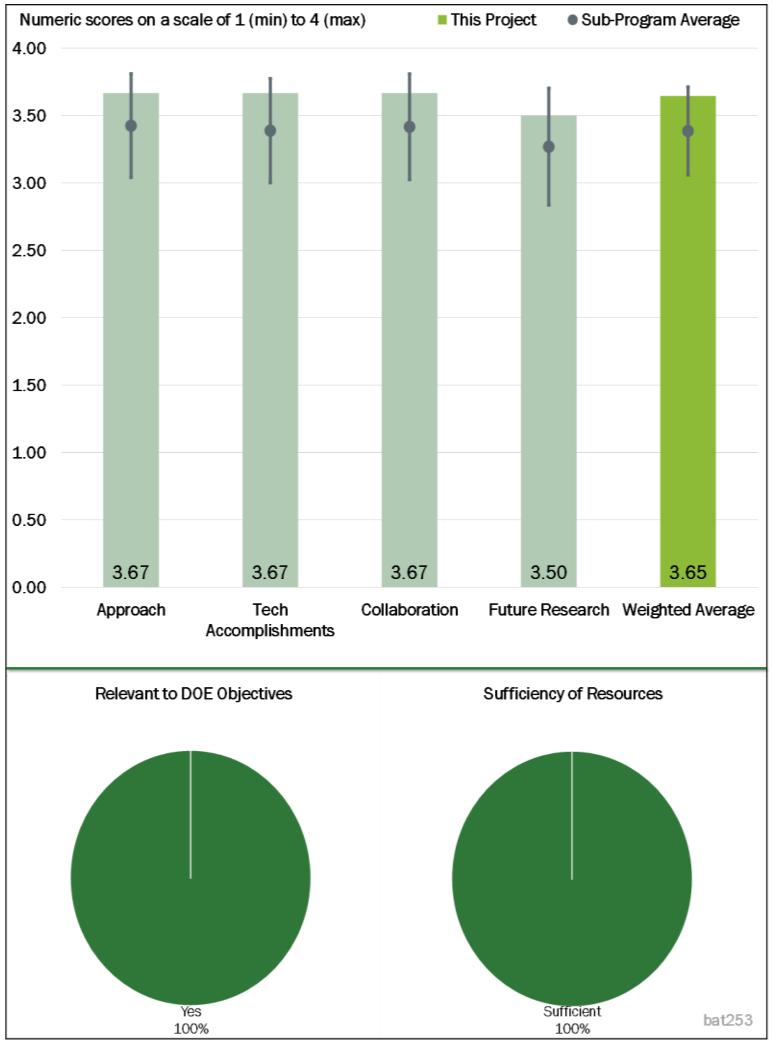

Figure 2-17 - Presentation Number: bat253 Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Theory and Modeling Principal Investigator: Hakim Iddir (Argonne National Laboratory)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer indicated that the project is both well-designed and well-executed with a sharp focus on details that impact NMC stability and interaction with the electrolyte. Experimental work complements the simulation approach, which keeps it reasonably grounded. The reviewer added even stronger support from experiment is desirable in the future.

Reviewer 2:

The reviewer stated that this program, related to fundamental modeling studies of complex battery materials issues, was well laid out and explained. The reviewer noted this is very complex work but the components of the program, including assumptions and limitations, was competently addressed. Comparisons of modeling outcomes versus experimental observation were an important part of the presentation.

Reviewer 3:

The reviewer explained that this project applied atomistic modeling approach for a theoretical prediction of the interfacial reactions between electrolyte and additive with cathode materials, which guide the design and synthesis of electrode material and electrolyte. This approach is highly linked with the real experimental work.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that this program has moved the ball forward with some legitimate comparisons of simplified particle models versus observed physical phenomenon. The question of whether the modeling can be predictive rather than confirming remains open; however, this is a solid base to continue work.

Reviewer 2:

The reviewer asserted that each individual topic is of interest to researchers working in the field and has produced novel conclusions. Particular emphasis is placed on TM segregation near surfaces and the mechanism of trimethoxypropylsilane (TMPSi) passivation on NMCs, which should be relevant for the future design of cathode coatings or electrolyte additives. The reviewer noted that if some of these conclusions can be generalized for a larger group of coating species (i.e., beyond alumina) or additives, it will be even more relevant for application.

Reviewer 3:

The reviewer remarked that this program meets a need by linking the experimental research and theoretical mechanism understanding, which is critical to design novel high-energy density, high-performance cathode materials for lithium ion batteries.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer emphatically described collaboration and coordination across the project team as outstanding and added that the strength of this project team is in its varied approaches and independent research topics that still hew to the theme of enabling higher energy cathode materials.

Reviewer 2:

The reviewer stated the appropriate level of collaboration appears to have been applied and that comparisons of modeling with experimental observation appear to have been well coordinated.

Reviewer 3:

The reviewer said this project was collaborated among many national laboratories and universities as showed in the presentation.

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

Reviewer 1:

The reviewer stated that overall the proposed future work is excellent. The reviewer suggested the PIs could pay more attention to link this project with the related experimental work in BAT 252 and BAT254 and show how this theoretical modeling can support those projects.

Reviewer 2:

Proposed future work was described as generally interesting by this reviewer, who expressed confidence in the researchers’ ability to extend these results by exploring other cathode surface interactions. The reviewer noted input from industry on relevant cathode coating materials (i.e., lithiated oxides) and processes (i.e., aqueous or non-aqueous sol gel) could be valuable to design simulations based on real systems, and exploring the impact of binder chemistry and location may also be interesting.

Reviewer 3:
Program direction appeared sound and in line with overall research from this reviewer's perspective.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer remarked that this project is very important and extremely relevant to DOE objectives to enable higher energy, longer cycle life cathode materials.

Reviewer 2:
The reviewer stated DOE's overall target is to develop Li-ion batteries with low cost, high energy density, and electrochemical properties, and this project's focus, modeling the interfacial reactions between electrolyte and high-energy density electrode materials, is consistent with DOE's goals.

Reviewer 3:
The reviewer asserted that developing a modeling component of complex materials behavior is relevant.

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

Reviewer 1:
The reviewer noted the resources from many national laboratories and universities are sufficient to support the research work of this project.

Reviewer 2:
The reviewer said the resources for this project are sufficient.

Reviewer 3:
The reviewer had no significant comment on resources.

Presentation Number: bat254
Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Materials Characterization
Principal Investigator: John Vaughey (Argonne National Laboratory)

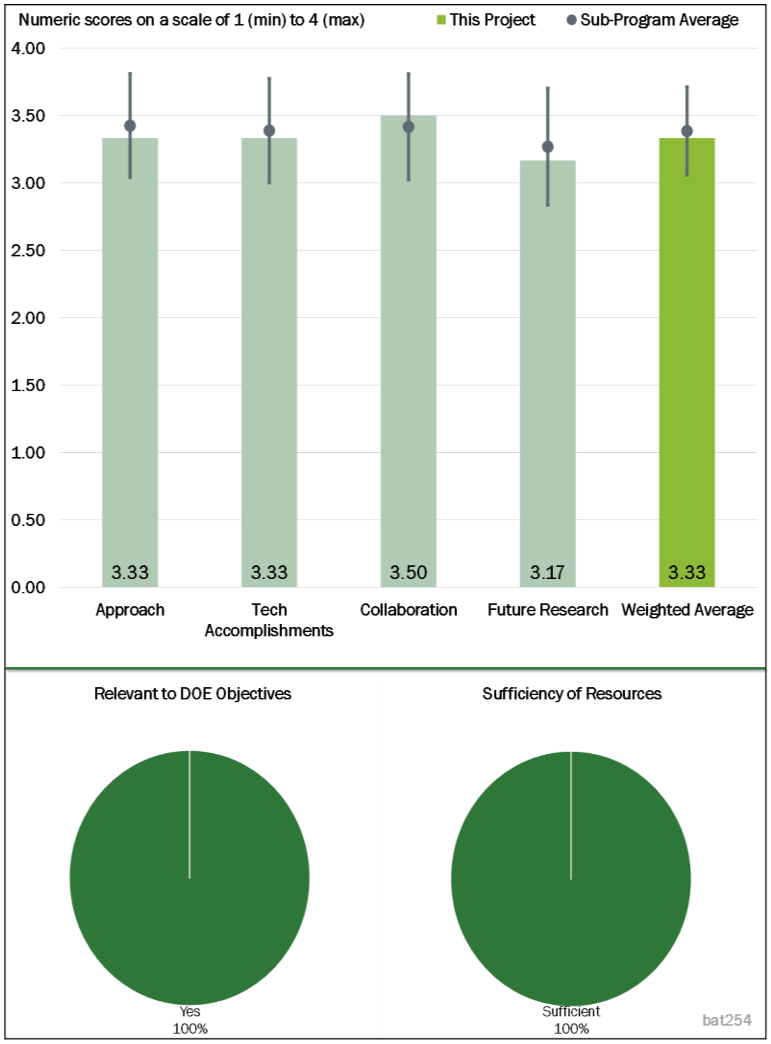

Figure 2-18 - Presentation Number: bat254 Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Materials Characterization Principal Investigator: John Vaughey (Argonne National Laboratory)

Presenter

John Vaughey, 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 and well-planned.

Reviewer 1:

The reviewer said the project is well-designed and well-executed with an interesting focus on understanding the role of alumina coatings on NMC cathode materials. The structure of various alumina coatings has been evaluated by solid-state NMR, electrochemistry and microscopy, revealing that the underlying composition of NMC (e.g., the concentration of Mn) is a critical variable in the coating structure and effectiveness. The effectiveness of annealing and original solution-based deposition method is also important to establish functionality. While the heavy use of NMR is informative, complementary surface science techniques, perhaps with depth profiling, would be helpful to confirm and understand changes in TM oxidation state. The development of thin film deposition techniques should allow these surface science studies in future work—but comparison to bulk synthesized particles may be a challenge.

Reviewer 2:

The reviewer stated the program sets out a reasonable goal of understanding and characterizing aluminum oxide (Al_2O_3) surface coatings on various NMC structures, which follows from a fairly well-known commercial use of this system in cobalt oxide systems. The reviewer added that, in general, this study takes the correct path toward characterization and understanding the differences between the two systems.

Reviewer 3:

The reviewer indicated that this project applied a wide array of characterization techniques as well as electrochemical models for a better understanding of the reaction mechanisms of high-energy density cathode materials in Li-ion batteries.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer described technical accomplishments and progress as excellent. It proceeds in a logical manner and the team used many characterization techniques to gain a full understanding of the structural information of the cathode materials with various doping/synthesis approaches and interfacial reaction with electrolyte. The reviewer said that all of the achievements are critical to realize the overall goals of the projects.

Reviewer 2:

The reviewer commented that results from the past year are valuable and will undoubtedly help in the design of new cathode coating materials or techniques. The reviewer added it would be useful to generalize these results for more than a single coating chemistry. The relationship of Mn concentration could be relevant to a subset of coating materials but not to others. Because other work in this area has also explored Ti, niobium (Nb), tantalum (Ta), etc. based coatings, broadening the type of coatings studied may be of commercial interest.

Reviewer 3:

The reviewer notes the outcome appears to be quite apparent that there are significant chemical differences in the way alumina interacts with the NMC systems. In particular, performance gains are neutral to negative, with performance trending down as higher Ni content materials are evaluated. The reviewer stated the proposed mechanisms for this appear reasonable.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer observed exceptionally strong collaboration across the project team.

Reviewer 2:

The reviewer stated the appropriate level of collaboration appears to have been applied and critical electrochemical testing of the systems was done appropriately.

Reviewer 3:

The reviewer indicated that this project was collaborated among many national laboratories and universities as shown in the presentation.

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 opined that suggestions for future work are interesting and could be valuable, particularly related to coating-electrolyte synergy. Further exploration of surface charge could be useful, but would have to be conducted using a new set of characterization techniques beyond NMR. In situ or operando (e.g., with electrolyte) studies of surface states would be most relevant, if possible.

Reviewer 2:

The reviewer noted the direction of the accomplished work seems to suggest that the alumina coating system is not necessarily a fundamentally compatibly system with the NMC systems under study. The reviewer added it seems that the team should give some careful thought to justify future directions this work might take on, and questioned is this system can be studied further as indicated or if other coating system be evaluated.

Reviewer 3:

The reviewer said the proposed future work is consistent with the current project direction, which should provide deeper and wider understanding of the high-voltage, high-energy density cathode materials.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer indicated that this project is very important and extremely relevant to DOE objectives to enable higher energy, longer cycle life cathode materials.

Reviewer 2:

The reviewer asserted that improvement of high-Ni NMC systems is very relevant to the DOE.

Reviewer 3:

The reviewer stated DOE's overall target is to develop Li-ion batteries with low-cost, high-energy density and electrochemical properties, and this project's focus, characterizing the interfacial reactions of high-energy density Ni-rich cathode material, is consistent with DOE's goals.

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

Reviewer 1:

The reviewer observed sufficient resources for this project.

Reviewer 2:

The reviewer noted sufficient resources from many national laboratories and universities to support the research work of this project.

Reviewer 3:

This reviewer had no significant comment.

Presentation Number: bat263
Presentation Title: Electrodeposition for Low-Cost, Water-Based Electrode Manufacturing
Principal Investigator: Stuart Hellring (PPG Industries)

Presenter

Stuart Hellring, PPG Industries

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 and well-planned.

Reviewer 1:

The reviewer observed a very good approach to developing an electrodeposition-based method for depositing Li-ion electrode suspensions onto current collectors.

Reviewer 2:

The reviewer indicated that the technical approach addressed battery production cost by developing thick electrode via aqueous processing.

Reviewer 3:

The reviewer noted minimal justification for this work other than concern regarding volatile organic compounds.

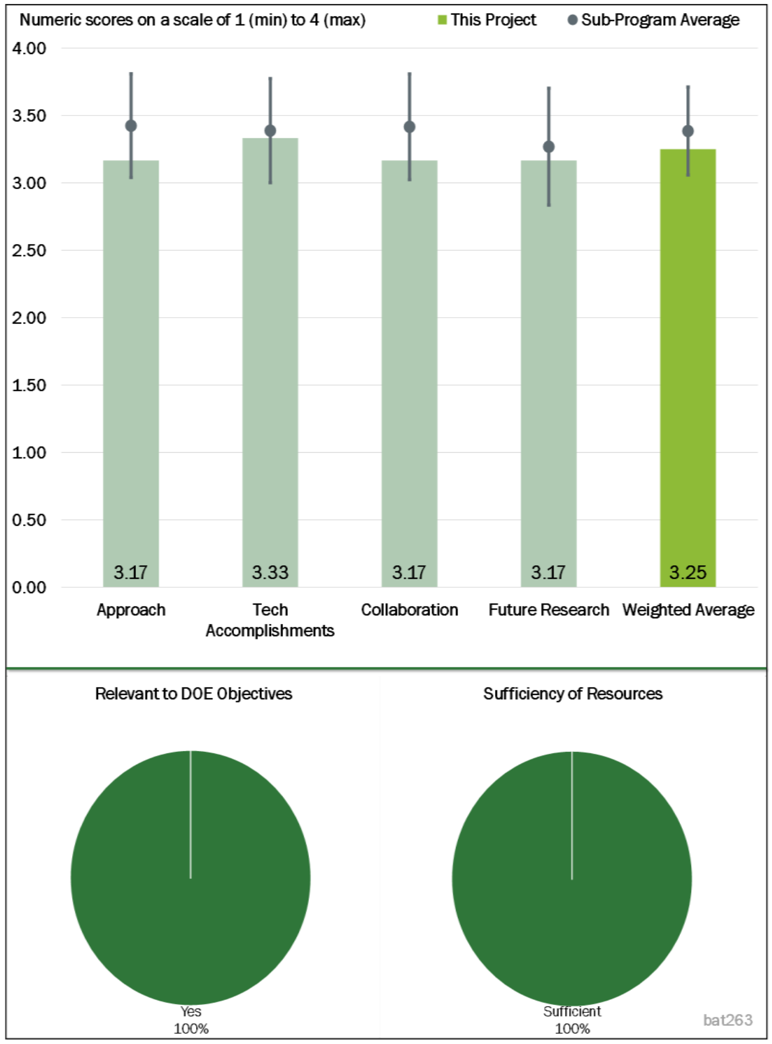

Figure 2-19 - Presentation Number: bat263 Presentation Title: Electrodeposition for Low-Cost, Water-Based Electrode Manufacturing Principal Investigator: Stuart Hellring (PPG Industries)

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted very good progress demonstrated to date. Really good and disruptive technology to replace slot dye coating methods, and to replace the toxic N-Methyl 2-Pyrrolidone (NMP) solvent with aqueous ones. The reviewer added the challenge is that one is still dependent on the same mix, coat, dry, calendar process. The only process step that is impacted is the coat step. Critically, this enables much thicker coatings, 2x that of NMP based solvent electrodes. This is important in that it gives us a new way to coat electrodes.

Reviewer 2:

The reviewer noted that, given the boundaries for this project, the project team established an excellent approach and the results of work yielded a level of success. However, the project team actually fails to indicate whether or not go/no-go state has been achieved. The reviewer stated that any work must have valid and specific metrics prior to funding a work-plan.

Reviewer 3:
The reviewer said the technical was made according to plan, although the production cost savings may be not huge.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted that PPG is working with ANL, ORNL, and Navitas, which is excellent. The reviewer encouraged PPG to collaborate with Lambda Tech to implement microwave assisted drying to make sure PPG has very good high loading electrodes—the Lambda tech drying approach is particularly valuable for thick electrodes.

Reviewer 2:
The reviewer described the partners as well-coordinated.

Reviewer 3:
The reviewer reported that an industrial partner is contributing to project. However, what is needed is whether this project is economically justified.

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:
In addition to the very relevant planned future research, this reviewer explained that the project should focus in the near-term on new capabilities that this technology could bring, such as controlled porosity, electrode structures for fast-charge, etc. The reason this reviewer mentioned this is because the reported cost savings of 1.8% at the cell level is almost certainly too little to entice a large call manufacturer to implement a brand-new technology.

Reviewer 2:
The reviewer commented that battery energy density appears to be more important than energy density for vehicle applications due to limited packing space, and that the project team may want to show the energy density of the cell with the new manufacturing processing compared to that of the base cell. The reviewer added that there are no explicit details about the uniformity of the electrode with the developed aqueous process.

Reviewer 3:
The reviewer observed a reasonable work-plan proposed by the project team, and suggested that it survey the industry at large to determine the best direction to take.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewed remarked that the project is very relevant in many areas of DOE technical roadmap.

Reviewer 2:
The reviews pointed out that the project supports the goals for battery manufacturing cost reduction.

Reviewer 3:
The reviewer noted the work meets DOE needs.

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 appropriate resources and added, it would be good or DOE to find a way to support this type of disruptive technology going forward.

Reviewer 2:
The reviewer noted the resources appear to be sufficient for the proposed efforts.

Reviewer 3:
The reviewer said yes.

Presentation Number: bat264
Presentation Title: Lithium-Ion Battery Anodes from Electrospun Nanoparticles/Conducting Polymer Nanofibers
Principal Investigator: Peter Pintauro (Vanderbilt University)

Presenter
Peter Pintauro, Vanderbilt University

Reviewer Sample Size
A total of three reviewers evaluated this project.

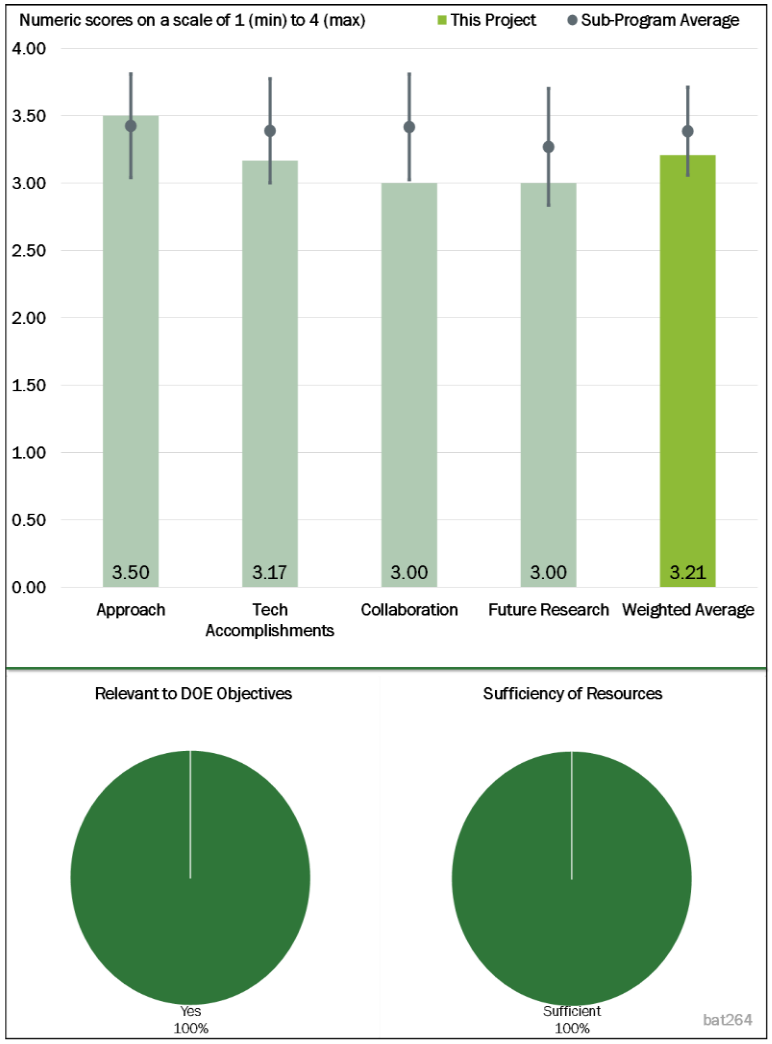

Figure 2-20 - Presentation Number: bat264 Presentation Title: Lithium-Ion Battery Anodes from Electrospun Nanoparticles/Conducting Polymer Nanofibers Principal Investigator: Peter Pintauro (Vanderbilt University)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer pronounced the approach to developing electrospun Si-based anodes to be good.

Reviewer 2:
The reviewer said that the technical approach addressed capacity-fade barriers for a Si anode-based, high-energy battery.

Reviewer 3:
The reviewer commented that the approach is both novel and presents an opportunity to achieve enhanced manufacturability of battery membrane composite structures.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer stated that the team has made significant progress towards its goals.

Reviewer 2:
The reviewer said that the technical progress is reasonable and aligns with the plan.

Reviewer 3:
The reviewer commented that the approach is not a bad way to manufacture Si-based anodes, but opined that there is just not a critical advantage here to convince the reviewer that this will be successful when other Si approaches have not been. The reviewer saw the biggest issue here as the lack of SEI stabilization with Si-

based anodes (see Slide 15). The other issue, more critical for consumer electronics applications, is volume expansion of the electrode, but this manufacturing approach does not address that either.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The collaboration across the team members appeared excellent to the reviewer.

Reviewer 2:
According to the reviewer, project assignments have been made and the team appears to communicate issues and results.

Reviewer 3:
The reviewer had no issue with collaboration, but suggested that it would be advantageous if Vanderbilt can determine how this approach can address the two main issues with SI-based anodes.

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

Reviewer 1:
The reviewer stated that the course is set to continue work. The team also needs to assess efforts made by other researchers outside of project team.

Reviewer 2:
The reviewer noted that battery energy density appears to be important for vehicle applications due to limited packing space. The reviewer suggested that the contractor may want to show the energy density of the cell with the new manufacturing processing compared to that of the base cell. The reviewer hoped to see more interactions with industry and a future plan for potential transition.

Reviewer 3:
The reviewer referenced prior comments.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
Enabling low-cost Si anodes is certainly relevant, according to the reviewer.

Reviewer 2:
The reviewer stated that the project supports the goals for an increase in battery specific-energy density.

Reviewer 3:
The reviewer remarked that advancements in energy storage are important to future energy developments.

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

Reviewer 1:
The resources appeared to be sufficient to the reviewer for this project.

Reviewer 2:
The reviewer stated that all is adequate.

Reviewer 3:
The reviewer thought that resources were okay.

Presentation Number: bat266
Presentation Title: Co-Extrusion (CoEx) for Cost Reduction of Advanced High-Energy and High-Power Battery Electrode Manufacturing
Principal Investigator: Ranjeet Rao (PARC)

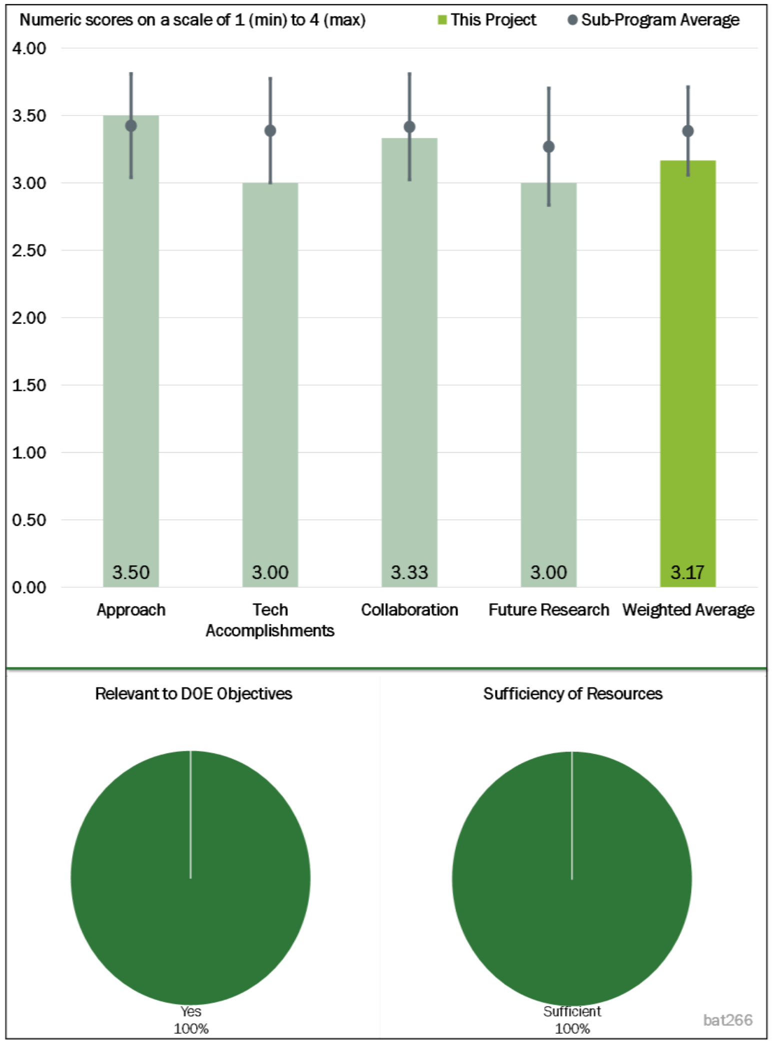

Figure 2-21 - Presentation Number: bat266 Presentation Title: Co-Extrusion (CoEx) for Cost Reduction of Advanced High-Energy and High-Power Battery Electrode Manufacturing Principal Investigator: Ranjeet Rao (PARC)

Presenter
Ranjeet Rao, PARC

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 and well-planned.

Reviewer 1:
The reviewer remarked that this is a very good approach for partially decoupling power from energy through novel, co-extruded, Li-ion electrode designs.

Reviewer 2:
The technical approach addressed battery production cost by developing thick electrodes via the co-extrusion method, according to the reviewer.

Reviewer 3:
The reviewer commented that the project seemed to duplicate efforts ongoing by others and may not yield expected results in any scale-up.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer stated that the technical approach sounds productive and the progress aligns with the plan. There is not sufficient detail outlined to support the cost-reduction claims.

Reviewer 2:
The reviewer said that progress is ongoing, but only minimal results have been reported.

Reviewer 3:
The reviewer commented that the structure shown on Slide 9 will likely result in rather minimal power improvement as the “thick” regions are almost a millimeter (mm) wide. The longest distance that charging and discharging reactions will take place in a high-power (3C-4C [charge rate of 3-4]) situation is less than 100

microns. These are five times that this can be seen in the extreme fast-charging program. Thus, the reviewer concluded that these “thick” pillars should probably be about 200 microns wide or less to ensure that Li ions are able to penetrate or escape the interior regions during high power pulses. Plots on Slides 11 and 12 show this. The reviewer said that the high rate behavior of the co-extrusion (CoEx) cathodes is better than the standard ones, but they are still losing 30%-50% of their C/10 capacity at 2C.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The collaboration across the team members appeared excellent to the reviewer.

Reviewer 2:
The reviewer saw good collaborations and had no issues.

Reviewer 3:
According to the reviewer, all participants seem to be fully involved.

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

Reviewer 1:
The reviewer was curious if an NMP-free process, such as that being studied at ORNL, can work together with CoEx for further cost reductions.

Reviewer 2:
The work plan has been established and the reviewer strongly suggested that the team create a dynamic model of “slurry” flow to better assess the likelihood of manufacturability of the reproducible electrodes at scale-up.

Reviewer 3:
The reviewer was concerned about the size of the “thick” cathode regions. The reviewer thought that they need to be much thinner. It will also be difficult to obtain good data if the anodes used in the cells are not fabricated to have similar power capability as the cathodes.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer stated that the project fits DOE’s mission scope.

Reviewer 2:
The reviewer noted that the project supports the goals for battery cost reduction and specific energy-density increases.

Reviewer 3:
The reviewer found the project to be extremely relevant as DOE is interested in enabling much thicker electrodes (for higher energy and lower cost cells) that still provide the needed power (for acceleration of the vehicle and fast-charge).

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

Reviewer 1:
Adequate resources are available, according to the reviewer.

Reviewer 2:

The reviewer said that the resources appear to be sufficient for the proposed efforts.

Reviewer 3:

The reviewer commented that the resources are reasonable. The reviewer supported DOE's finding a way for further funding to PARC to extend this approach to the anode and to thin the width of the thick regions.

Presentation Number: bat269
Presentation Title: An Integrated Flame-Spray Process for Low-Cost Production of Battery Materials
Principal Investigator: Chad Xing (University of Missouri)

Presenter
Chad Xing, University of Missouri

Reviewer Sample Size
A total of three reviewers evaluated this project.

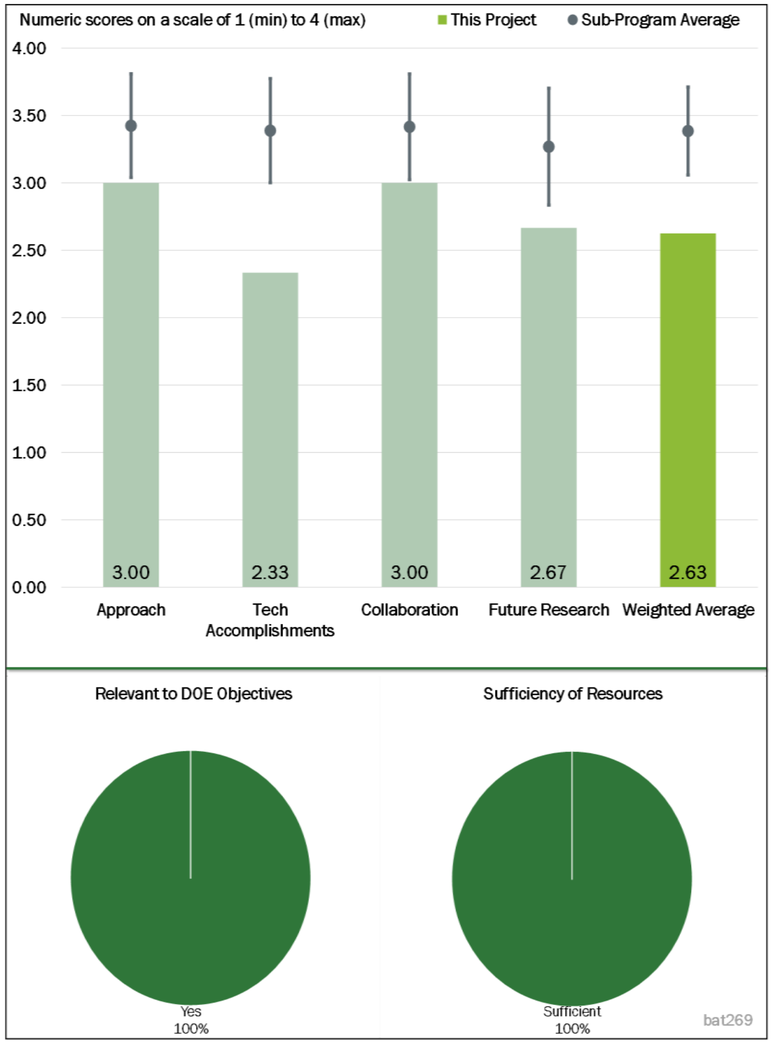

Figure 2-22 - Presentation Number: bat269 Presentation Title: An Integrated Flame-Spray Process for Low-Cost Production of Battery Materials Principal Investigator: Chad Xing (University of Missouri)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer noted that the technical approach addressed battery production cost by developing thick electrodes via an integrated flames spray process.

Reviewer 2:
The reviewer said that it is reasonable to consider novel ways to make Li-ion electrodes.

Reviewer 3:
According to the reviewer, flame spray is historically an inconsistent process with considerable waste. This, combined with issue of Li vapor pressure, raises concerns regarding process viability at scale-up for manufacturing.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer found the technical progress to be reasonable though some milestones were delayed due to a major change in the flame reactor.

Reviewer 2:
The reviewer stated that the reported successes have been few. Also, the team reports need to re-evaluate go/no-go milestones involving past work.

Reviewer 3:
The reviewer remarked that there has been a very rough start to this program due to major issues with active material capacity, density, and now cell-cycle life. The team has recently increased its beginning of life (BOL)

capacity to near commercial levels, which is good, but Slide 9 shows a 30% fade in 50 cycles, which is incredibly bad.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted that the team has designated partner assignments. Communication of work is ongoing among the team members.

Reviewer 2:

The reviewer stated that the contractor has put together a team consisting of academia and industry partners collaborating to attack the technical barriers. A future collaboration with academia, including national laboratories, is expected

Reviewer 3:

It seemed to the reviewer that this team needs help perhaps with electrode fabrication or cell construction. Eagle Picher is currently not participating at all, which may be holding the team back. The reviewer suggested trying to engage with a national laboratory electrode and cell-building team.

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

Reviewer 1:

The reviewer mentioned that the team is simply continuing its effort based on the original work plan without extensive modification from lessons learned.

Reviewer 2:

The reviewer hoped to have seen the stability comparison for the materials produced with the developed method and the baseline materials and was curious if the process being developed can be applied to other battery materials oxides, such as LFP and LTO.

Reviewer 3:

Referring to Slide 12, the reviewer suggested not spending time and money on surface coatings until the bare NMC can perform as well as commercial powders. The coating just complicates interpretation of what is causing poor performance. Currently commercial NMC cells can cycle hundreds of times at the voltages used here. To remove the maximum voltage (V_{max}) from the fade mechanism, the reviewer urged that these cells be tested at a more reasonable 4.3V and demonstrate acceptable cycle life.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer had no issue with relevance.

Reviewer 2:

The reviewer stated that the project supports the goals for battery cost reduction.

Reviewer 3:

The reviewer remarked that battery development is with DOE mission scope.

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

Reviewer 1:
The reviewer had no issue with resources.

Reviewer 2:
The reviewer said that the resources appear to be sufficient for the proposed efforts.

Reviewer 3:
The resources appeared to be adequate to the reviewer.

Presentation Number: bat273
Presentation Title: Composite Electrolyte to Stabilize Metallic Lithium Anodes
Principal Investigator: Nancy Dudney (Oak Ridge National Laboratory)

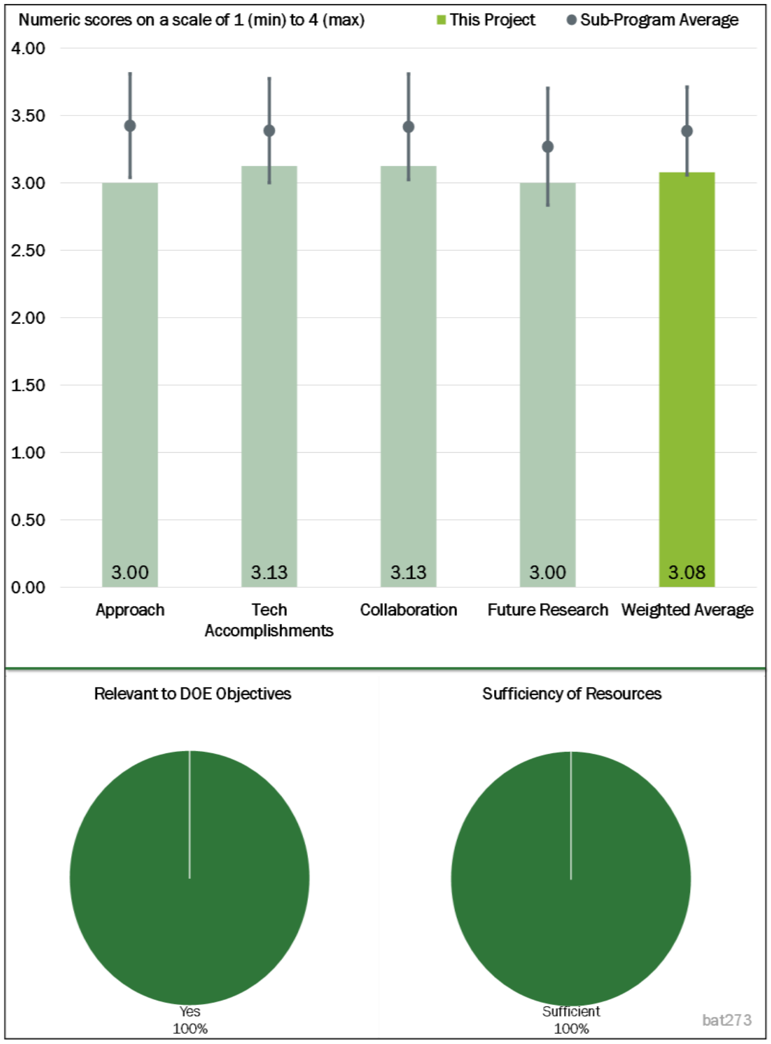

Figure 2-23 - Presentation Number: bat273 Presentation Title: Composite Electrolyte to Stabilize Metallic Lithium Anodes Principal Investigator: Nancy Dudney (Oak Ridge National Laboratory)

Presenter

Xi Chen, 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 and well-planned.

Reviewer 1:

The reviewer stated that a composite electrolyte is a good way to protect a Li anode. The project approaches the goals from multiple angles and addresses the safety and efficiency barriers of Li-metal.

Reviewer 2:

The reviewer noted that the approach taken is a logical research effort for overcoming the technical barriers for Li-metal. The group is concentrating on the major factors impeding a stable electrode. The team is focusing on improving room-temperature ionic conductivity and the low-shear modulus of polymer electrolytes. The reviewer said there were efforts to include a comparison with Ohara ceramics, which is good. Identifying a suitable SSE for Li-metal anodes is paramount in order to meet VTO goals.

Reviewer 3:

The reviewer pointed out that the objective of this multi-year project is to mitigate the problems of poor cycle life, safety, and reliability with the Li-metal anode, which can potentially contribute to much higher energy densities in cells containing high-capacity cathodes (Li-sulfur or Li-air cells) through using solid-polymer electrolytes in lieu of conventional liquid electrolytes. While polymer electrolytes have advantages in electrochemical stability (with Li) and processability, ceramic electrolytes have the advantage of having a high sheer modulus. The reviewer indicated that this project is focused on developing composite solid electrolytes based on both, which however would also need an interfacial layer (in this case a polymer). Specifically, the reviewer noted that the composite solid electrolyte investigated here includes an Ohara Corporation ceramic electrolyte in high proportion blended with polyethyleneoxide (PEO)-based polymer electrolytes with a plasticizer. There is considerable contact resistance between the polymer and ceramic electrolytes, which, though reduced marginally with the use of plasticizer, is still a challenge. The reviewer did not find much novelty in this approach (a few other researchers dabbled with this approach), which is cumbersome process-wise with triple layers, and the results here are not outstanding or promising yet after as many years. Nevertheless, based on the difficulties associated with all solid-electrolyte systems, this may be a viable approach. Thus, the reviewer concluded that this project is well integrated with the other DOE VTO projects and consistent with its goals towards high specific energy density of 500 Wh/kg at the cell level.

Reviewer 4:
The reviewer said that the solid electrolyte using polymer and ceramic composite seems working, but the internal resistance is quite high. Probably because of this, no study has been done nor planned for observing Li-dendrite formation, although it is a very important barrier.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer stated that significant accomplishments were made this year. The density of the membranes was improved by a new technique. The group published a paper in the *Journal of Power Sources.*

Reviewer 2:
The reviewer remarked that fairly good progress has been made in developing composite solid electrolytes based on PEO and an Ohara glassy electrolyte with a high proportion of solid electrolyte. The composite membrane formed by aqueous spray coating and hot pressing was found to have high density and also a high Li-transference number (compared to the polymer electrolyte). However, the reviewer commented that these composite electrolytes ended up having high contact resistance between the ceramic and polymer electrolyte, more than the bulk resistance of either polymer or solid electrolyte even with a plasticizer. The reviewer pointed out that the contact-resistance issues are no less challenging in all solid-electrolyte systems. Possibly new polymer and ceramic systems with low interfacial area-specific resistance (ASR) need to emerge to have this approach meaningful or successful. Possibly other solid electrolytes (e.g., Li lanthanum zirconate [LLZO]) with better interfacial compatibility with lithium than Ohara, could have been attempted here. Overall, the progress here is good and directed towards DOE goals of high specific energy by enabling the use of a Li-metal anode.

Reviewer 3:
The reviewer said that some results were obtained, but the ion conductivity is quite low.

Reviewer 4:
The reviewer stated that spray coating the cathode followed by the composite electrolyte shows great improvement for this Li-anode system; tri-layer cells and a tetraethylenegylcoldimethyl (TEGDME) composite electrolyte showed some promising results and can be further developed. However, all solid, full-cell performance improvement is still based on cycling at high temperature, which is also the limitation for this technology. The reviewer commented that a lot of electrochemical measurements have been performed in this project, which can provide good guidance for interfacial studies.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
According to the reviewer, there are good collaborations with researchers from ORNL, a university (Michigan State University), and industry (Ohara).

Reviewer 2:
The reviewer commented that collaboration with more agencies than last year can be seen in terms of materials preparation and characterization.

Reviewer 3:

The reviewer remarked that there is good collaboration with other laboratories. These include Jeff Sakamoto (Michigan State University), Ohara, and polymer researchers at ORNL.

Reviewer 4:

The reviewer suggested that the collaboration should be extended to accelerate the project with a stronger connection with both universities and national laboratories.

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

Reviewer 1:

The reviewer noticed that the PI knows what she is doing and this is a pretty long program, which started in 2014.

Reviewer 2:

The reviewer found the proposed efforts to be realistic and appropriate. Minimizing interfacial resistance is critical. Moving toward a polymer gel is a realistic approach.

Reviewer 3:

The reviewer noted that there are still quite a few outstanding technical barriers in the development of composite solid-polymer electrolytes that are stable with a Li anode with low interfacial resistance (ASR). The proposed future studies of assessing new chemical and mechanical treatments of the Li interface with a composite electrolyte, examining new polymer/solid electrolyte combinations, adopting a barrier layer (Li phosphorous oxy-nitride [LiPON]) over a composite polymer electrolyte to stabilize the plasticizer, and developing full cell designs by spray coating these composite membranes with higher ceramic loading with bimodal particle sizes are logical and address the key technical barriers towards using Li-metal anodes. The reviewer said that these studies are consistent with the DOE goals of high specific energy.

Reviewer 4:

The PI should try materials beyond Ohara and PEO, which is very necessary because they have been shown limited potentials. However, the PI does not specify what are the alternative materials are. The reviewer mentioned that the size of particles may be a factor but should not be too critical.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that if this project can be successful in the next few years, the impact will be huge for the field of high-energy batteries.

Reviewer 2:

The reviewer stated that this project supports DOE objectives. The types of electrolytes that the team is developing may enable using Li-metal anode, allowing for batteries with higher energy densities and enhanced safety.

Reviewer 3:

The reviewer explained that for the widespread use of EVs, the batteries need to be lightweight, compact, safe, and low cost. The state-of-the-art Li-ion batteries are inadequate to fulfil these needs. Higher specific energy density (at least 500 Wh/kg) and lower cost batteries are being developed by DOE, either with Ni-rich NMC cathodes or sulfur cathodes that needs integrating with stable Li anodes. The reviewer commented that a long-life Li anode is desired to meet the DOE goals, which this project has been addressing by aiming to develop suitable composite solid polymer electrolytes.

Reviewer 4:
The reviewer remarked that finding proper solid or composite electrolytes would definitely be a good use of Li and the anode. This should give higher capacity than a 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 reviewer remarked that the resources were adequate for the scope of the project.

Reviewer 2:
The resources for this project are sufficient, according to the reviewer.

Reviewer 3:
The reviewer noted that the project has sufficient funding and resources to successfully complete the milestones.

Reviewer 4:
Although no financial data were reported, the reviewer assumed that funding is sufficient.

Presentation Number: bat282
Presentation Title: Development of High-Energy Lithium-Sulfur Batteries
Principal Investigator: Jun Liu (Pacific Northwest National Laboratory)

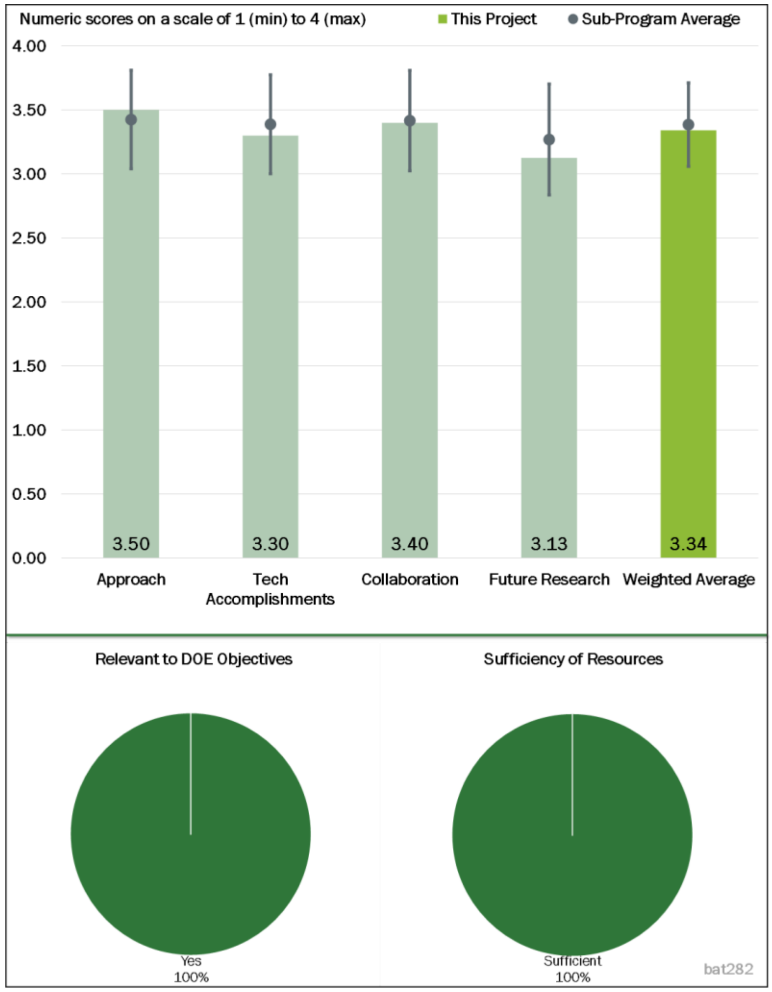

Figure 2-24 - Presentation Number: bat282 Presentation Title: Development of High-Energy Lithium-Sulfur Batteries Principal Investigator: Jun Liu (Pacific Northwest National Laboratory)

Presenter

Dongping Lu, Pacific Northwest 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 and well-planned.

Reviewer 1:

The reviewer commented that the PNNL team has done excellent work in studying high-energy Li-sulfur batteries. The team unveiled the effects of electrode porosity control on cell energy, sulfur utilization, electrolyte-sulfur ratio and cell-cycling life. The progress advanced the fundamental understanding of electrolyte-additive degradation mechanism in Li-sulfur batteries. The study on sulfur cathodes, by completely decoupling the interferences from lithium anodes, is innovative. The reviewer remarked that the project has made remarkable progress in addressing the technical barriers.

Reviewer 2:

The reviewer praised the good approaches for overcoming barriers of Li-sulfur batteries, including high sulfur loading, Li-anode degradation, and lithium nitrate ($LiNO_3$) depletion. The strategies seem very well designed and are feasible to the reviewer.

Reviewer 3:

According to the reviewer, the development of high-loading sulfur cathodes is a critical step for advancing Li-sulfur battery technology. The additive/binder modification by PNNL is effective and produced good results in improving the sulfur utilization ratio, thereby improving the output capacity of the cathode.

Reviewer 4:

The reviewer stated that the approach of the project is well-structured and focused on some of the key problems of Li-sulfur systems.

Reviewer 5:
The approach seemed fine to the reviewer, who wanted to see the team explain and identify some fundamental interactions that may lead to further improvements. Li-sulfur has some pretty complicated chemistry going on.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer commented that the PNNL team has demonstrated several significant technical accomplishments and progress in the overall project. The project is in good shape in terms of milestones.

Reviewer 2:
According to the reviewer, the project is contributing to overcoming important barriers of Li-sulfur batteries, including high sulfur loading, low electrolyte/sulfur (E/S) ratio, and $LiNO_3$ problems. While contributions have been made to solving these problems, work remains to done on performance issues, such as cycle life and E/S ratio that are still not very good. The author did not report much on electrolytes for Li-sulfur batteries, which is very important.

Reviewer 3:
The reviewer stated that the project team demonstrated solid accomplishments on both the cathode and separator, which is excellent. Increasing porosity is a rather trivial improvement but a necessary step. The reviewer suggested that the team identify the exact mechanism besides increased specific area that leads to cathode improvement. The reviewer posited that the mechanism may involve higher order polysulfide chains and rings maybe filtered by pores.

Reviewer 4:
The reviewer indicated that the group has identified several degradation and performance issue effects in the sulfur cathode, which contributed to the deciphering of degradation mechanisms on these surface. However, several of these efforts seem to be stand-alone projects; e.g., a combination of electrode porosity structuring with electrolyte wetting additives could achieve better performance results and provide new insights on degradation effects at the electrode level.

Reviewer 5:
The reviewer said that the project developed high sulfur-loading cathodes that showed good capacity and cycling stability. The only concern the reviewer had is the bulky cell format. A more practical cell format will need to be developed or proposed in the program, and eventually, a kWh/kg cell should be presented as one of the final performance parameters.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the team has been collaborating with BNL, University of Wisconsin at Milwaukee, and General Motors (GM). The collaboration is very productive.

Reviewer 2:
The reviewer indicated that the project has a very good team and good collaborations.

Reviewer 3:
The reviewer commented that the team at PNNL seems reasonably well integrated into the research network; maybe one or two additional partner building up cells with these technologies should be added. Industry partners could contribute to define the energy and performance targets at the cell level.

Reviewer 4:

The reviewer remarked that good collaboration across the teams was demonstrated on this project. For the best result, however, a separator team will help the project very positively.

Reviewer 5:

The reviewer wanted to have seen more involvement from GM. The team should be running multiple samples and demonstrating statistically significant experimental results with error bars. It looked to the reviewer like the team applied some pretty standard electrochemical energy storage (EES) measurements for some battery. The reviewer saw an outlier point in the figure on Slide 15. The reviewer would like to have seen a little more from the industrial collaborators.

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

Reviewer 1:

The reviewer noted that the proposed future work is well planned. The team will focus on several key tasks, such as new cathode additives, electrode preparation methods, rational electrode architectures to enable high sulfur utilization (greater than 1,100 milliampere-hours/gram [mAh/g]) under conditions of high loading (more than 6 milligrams/square centimeter [mg/cm$^{2]}$), and dense electrodes (more than 1 gram/cubic centimeter [g/cc]). The proposed roadmap is very thoughtful and makes sense.

Reviewer 2:

The reviewer noted that the Overview Slide for the project indicates that the project ends in September 2018, but the Future Work Slide shows 2018-19. It was unclear to the reviewer if the project is ending. The Future Work slide seems generally good, but the author could place more emphasis on the electrolyte.

Reviewer 3:

In general, the proposed future work sounded reasonable to the reviewer; however, the project could benefit from a stronger combination of results and approaches towards an optimized cathode architecture that could provide interfacial stability at the electrode level. The targets of the project could be also defined on the cell level rather than the materials level to increase applicability.

Reviewer 4:

The reviewer opined that good future work was proposed only to satisfy the original work plan and objectives. A more practical energy-density target, using a kWh/kg-cell, should be included as one of the project goals.

Reviewer 5:

The reviewer agreed with trying to understand the fundamentals. Again, the chemistry is significantly more difficult that traditional Li-ion chemistry. The reviewer would like to have seen the PI identify some fundamental interactions that could lead to improvements. The additive that leads to increased porosity is okay, but an additivity that influences the chemistry is more interesting and useful to the community. The reviewer also suggested that the University of Wisconsin look at what electrolytes may improve performance. There was no mention of the electrolyte used. The reviewer also wanted to see GM running more than one sample. Also, the reviewer asked the team to add error bars to the experimental data. This is extremely important for conveying the significance of new data.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said yes, as the project does support overall DOE objectives because Li-sulfur is a high priority.

Reviewer 2:
According to the reviewer, removing the barriers of low practical energy density, shuttle effect, low rate capability, and limited cycling life is critical for commercialization of Li-sulfur batteries and highly relevant to the VTO goal.

Reviewer 3:
The reviewer responded affirmatively that Li-sulfur cells are a potential new technology for electric transportation and/or energy storage.

Reviewer 4:
Research and development on high energy-density Li-sulfur battery technology supports overall DOE objectives.

Reviewer 5:
The reviewer stated that there was excellent relevance.

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

Reviewer 1:
The reviewer noted that the team has fully used the resources at PNNL, BNL, University of Wisconsin at Milwaukee, and GM through collaboration.

Reviewer 2:
The reviewed remarked that the current resources are sufficient to achieve the project goals.

Reviewer 3:
According to the reviewer, current resources for this project are sufficient to achieve the stated project milestones.

Reviewer 4:
The reviewer indicated that the resources are sufficient.

Reviewer 5:
Resources seemed fine to the reviewer, who suggested requiring GM to run more samples using their resources.

Presentation Number: bat293
Presentation Title: A Closed-Loop Process for End-of-Life Electric Vehicle Lithium-Ion Batteries
Principal Investigator: Yan Wang (WPI)

Presenter

Yan Wang, WPI

Reviewer Sample Size

A total of four reviewers evaluated this project.

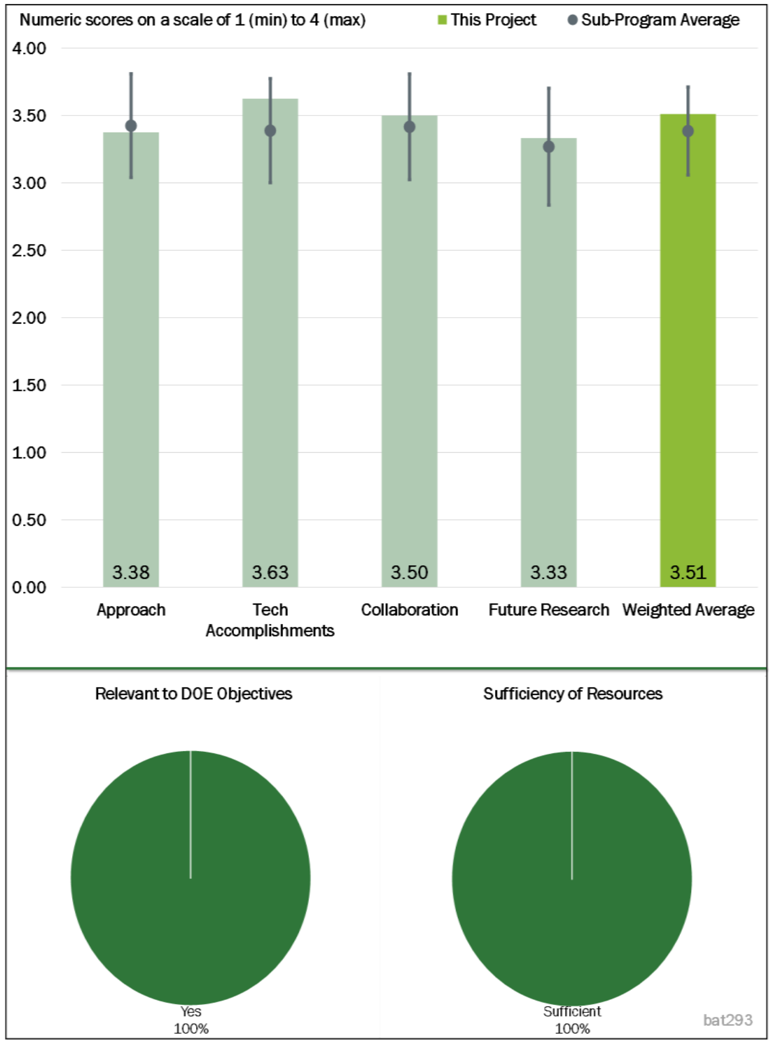

Figure 2-25 - Presentation Number: bat293 Presentation Title: A Closed-Loop Process for End-of-Life Electric Vehicle Lithium-Ion Batteries Principal Investigator: Yan Wang (WPI)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer pronounced the approach to be great, and stated that there was a well-organized plan. The reviewer thought that the idea of turning everything into NMC (111) is a great one. The reviewer was impressed.

Reviewer 2:

The reviewer pointed out that recovering more than 90% of materials from Li-ion batteries has not been achieved in other processes; also, shredding is more efficient than burning. However, more information is required as to the quality of the materials. The reviewer asked what tests have been performed on the final products. The opinion of the reviewer was that more electrochemical testing and cost-effective studies are required to define the economic feasibility of the project.

Reviewer 3:

The reviewer would have liked some discussion on how the technology would be commercially viable as electrodes become better and better and cells last longer.

Reviewer 4:

The reviewer found the approach to be okay, but the target sort of moved over the course of the program. In retrospect, the program should have addressed the robustness of the process to changes in feed stream or changes in the Ni ratio in the resulting precursors. The precursors critical to quality characteristics were not clearly stated and may not have been thoroughly addressed. The reviewer commented that the impact of cell SOH and robustness to commingling cathode chemistries/surface-treated cathodes or even variations from suppliers should have been addressed.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
Their accomplishments are terrific, according to the reviewer.

Reviewer 2:
With the limitations of academic R&D facilities and access to supplier information and requirements, the reviewer noted that the program accomplishments should be recognized.

Reviewer 3:
The reviewer observed that most of the items to be developed have been finished on time. Scaling up to commercialization level could be improved, following the indicators of the pilot plant (operational in summer 2018).

Reviewer 4:
The reviewer thought that there needs to be more investigation of cells to avoid hero cell syndrome.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer reported that the team has an impressive list of collaborators, including all three U.S. carmakers.

Reviewer 2:
The reviewer noted that several private companies contribute with samples of batteries, and the team has a partnership with one national laboratory. This collaboration and partners are present throughout the project so work is being performed under collaborations. The team has several sources of end-of-life EV batteries and specialized centers to perform tests.

Reviewer 3:
The reviewer commented that there was a good selection of teams, but the reviewer was not sure about the total interactions as some appear stronger than others.

Reviewer 4:
The reviewer pointed out that collaboration and coordination were better than average, but strong electrode active material suppliers were lacking.

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

Reviewer 1:
The reviewer said that all of the important goals are in their plans. There were no specific ideas presented for how the team will overcome whatever challenges remain.

Reviewer 2:
The reviewer observed that diagrams show a plan based on the results obtained earlier. There are no alternative pathways that could be followed now that the project has ended.

Reviewer 3:
The reviewer opined that there needed to be a discussion of viability of technology as materials improve and cells last longer. Also, there was a need to evaluate the introduction of higher Ni content and other anodes.

Reviewer 4:
The reviewer stated that the project has ended.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer found the project to be tremendously important for the long-term viability of Li-battery technology.

Reviewer 2:
The reviewed stated that this project supports overall DOE goals. The fabrication of commercial cells from recycled materials could reduce costs and mitigate environmental damage of end-of-life EV batteries.

Reviewer 3:
Reducing and recycling Co is a DOE priority, according to the reviewer.

Reviewer 4:
The reviewer remarked that recovering Co imports is relevant to vehicle electrification, and recovery/recycling should be evaluated. The reviewer said that the project would be more relevant with a discussion of harvesting the active materials, dealing with the recycling process waste streams, and the potential for process intensification.

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 resources are okay.

Reviewer 2:
Resources looked fine to the reviewer.

Reviewer 3:
The reviewer noted that milestones were met on schedule and budget.

Reviewer 4:
The reviewer found the resources for the project to be sufficient. Additional costs had not been reported. Due to tasks that are sequential, more resources do not mean that the milestones would have been achieved in less time. The manufacture of large batteries from recycled material demands the progressive fulfillment of scaling.

Presentation Number: bat296
Presentation Title: Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries
Principal Investigator: Chulheung Bae (Ford)

Presenter
Chulheung Bae, Ford

Reviewer Sample Size
A total of five reviewers evaluated this project.

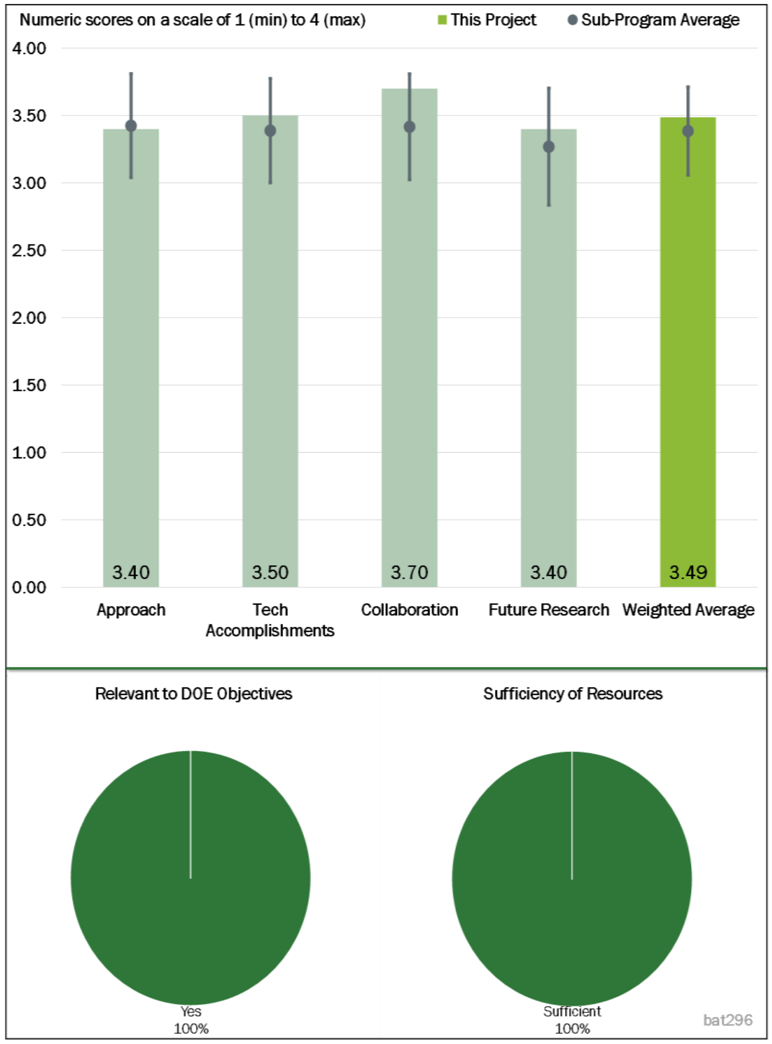

Figure 2-26 - Presentation Number: bat296 Presentation Title: Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries Principal Investigator: Chulheung Bae (Ford)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer indicated that this is a good start to the challenges of mechanical-abuse modeling of Li-ion batteries. The tasks are manageable and will add up to a potentially useful tool for the simulation of mechanical failures.

Reviewer 2:
The reviewer noted that the PI’s team has addressed most raised batteries, including the reduction of development cost and the improvement in the abuse tolerance. The project is well designed and feasible.

Reviewer 3:
The reviewer offered that researchers addressed the technical barrier very well with the developed simulation tool. Long simulation time is one of the barriers in battery simulation and the method developed will help to reduce the simulation time, keeping the accuracy.

Reviewer 4:
This project aims to provide electrochemical properties, such as ionic diffusivity, and conductivity as input data for multiphysics simulation tool developed in another project. In addition, a correlation between electrode thickness and SOC was achieved in initial cycles with slow charging. The technical barriers are addressed clearly.

Reviewer 5:

The approach seemed fine to the reviewer, who suggested using a combined thick- and solid-shell approach. The thick shell could be used for the extremely thin layers and solid elements for the materials with larger thickness. Treating everything as a single thick shell means that separation of the layers cannot be considered. This seems like a critical aspect because not all layers are perfectly adhered to each other. The reviewer would like to have seen more experimental results as it looks as if the team ran only three trials for each loading. The reviewer opined that this is a pretty straightforward test on the Angstrom machine. The reviewer would like to have seen at least 16 trials.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

According to the reviewer, the methodical development used in the technical accomplishments is well defined with define, develop, validate, and calibrate approach.

Reviewer 2:

The reviewer found the technical accomplishments and progress towards overall project to be excellent. The layered solid-element solver was further developed and calibrated with various materials models. Electromagnetic (EM) and thermal models were developed and calibrated. A new solver and an α-version multiphysics model were developed and verified with empirical data from these tests.

Reviewer 3:

The reviewer said that the accomplishments were good. It seemed to the reviewer the team has a working model that runs in a reasonable amount of wall time.

Reviewer 4:

According to the timing given in the poster, the reviewer remarked that the project has been successfully meeting its milestones with the delivery of the alpha version of the model.

Reviewer 5:

The reviewer reported that that most barriers have been effectively solved, the layered solid-element solver was developed, EM and thermal models were developed and calibrated, and a multi-physics model was developed and verified with empirical data from the following tests. However, the reviewer had two questions. In the development of the layered solid solver, the anodes and cathodes are represented by the same model, MAT-63. However, the physical and electrochemical properties for the anode and cathode may vary a lot. The reviewer asked if it is possible to develop different models for different materials. For the model to evaluate the performance of layered solid elements in EM and thermal solvers, the reviewer wanted to know if the cell deformation of the internal short-circuited cells plays an important role and should be considered. In Slide 21, the reviewer could not find a clear difference between the standard and layered solid elements and asked for a detailed explanation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found to work to be very well coordinated with DOE national laboratories for fundamental research aspects and coupled with software developer to implement the software tool necessary to carry out the project.

Reviewer 2:

The reviewer remarked that this project is a very good collaboration between industry and the national laboratories on a problem relevant to the development of battery electric vehicles.

Reviewer 3:

The reviewer noted that both ORNL and LS-DYNA participate in the project, and are well coordinated.

Reviewer 4:

The reviewer commented that the partners participate and are well coordinated.

Reviewer 5:

Collaboration seemed fine to the reviewer, who wanted the team to seek collaboration with a DOE high-performance computing (HPC) center. The mesh count could be higher. LS-DYNA scales extremely well across processors. The team should try to keep the cell count upwards of a million cells and then run across multiple processors on the HPC system. The reviewer had several suggestions: asking Ford to speed up their testing method, conducting more experimental trials, looking into what is going on with boron nitride, and putting down a poly(tetrafluoroethylene) (PTFE) sheet and carrying on if sticking is to be avoided.

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 well-thought out plans for future research. The addition of a durability assessment certainly benefits the overall development process.

Reviewer 2:

The reviewer stated that the proposed future research, including milestones and risk management, is logical.

Reviewer 3:

The reviewer supported the new experimental testing facility and the impact-based testing. The reviewer also suggested multiple pack testing. The reviewer noted that in the multipack scenario, some of the pack see a shear failure while others see a tension-tearing failure. The multi-stack configuration should be modeled to predict both of these failures.

Reviewer 4:

The reviewer commented that the cell testing data are very interesting, but in a real-world situation, the cells will be in a module configuration and may not experience mechanical abuse in the same way. The next phase of the project should emphasize module level testing/modeling.

Reviewer 5:

The reviewer reported that the PI's team has proposed clear future research goals, which are testing the beta-version model validation and high-speed impact. These tests are effective to realize the project target, which is to predict the combined structural, electrical, electrochemical, and thermal responses of batteries. However, the overcharge issue has not been mentioned in the report.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer stated that the team has met performance objectives, addressed barriers, there are well-defined partners for collaboration, and all deliverables in the matrix have been completed on time.

Reviewer 2:

According to the reviewer, this project supports the overall DOE objectives. Developing a simulation tool to predict the combined structural, electrical, electrochemical, and thermal (EET) responses of automotive batteries could improve their performance and reduce the cost of the vehicles.

Reviewer 3:
The reviewer found the relevance to be excellent.

Reviewer 4:
The reviewer affirmed that this project should help with the development of safe electric vehicles.

Reviewer 5:
The reviewer commented that this project supports the overall DOE objectives because the prediction of battery safety is important and necessary for the development of high-energy and low-cost 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 remarked that the resources seem appropriate for this program. More funding may be needed for module-level abuse testing.

Reviewer 2:
The reviewer stated that the research team has sufficient funding, human resources, and equipment to complete the project.

Reviewer 3:
The reviewer said that the partners were chosen for understanding the fundamentals as was the software developer for simulation tools that help to achieve the timely deliverables.

Reviewer 4:
Resources seemed good to the reviewer, who suggested that the team should be using a HPC system. The reviewer commended the attempt to find a new experimental test facility that has better throughput.

Reviewer 5:
The reviewer commented that the resources are sufficient to achieve the stated milestones in a timely fashion. A proper supplier to run material analyses for the beta-version, model-validation tests is very necessary.

Presentation Number: bat298
Presentation Title: Efficient Simulation and Abuse Modeling of Mechanical-Electrochemical-Thermal Phenomena in Lithium-Ion Batteries
Principal Investigator: Shriram Santhanagopalan (National Renewable Energy Laboratory)

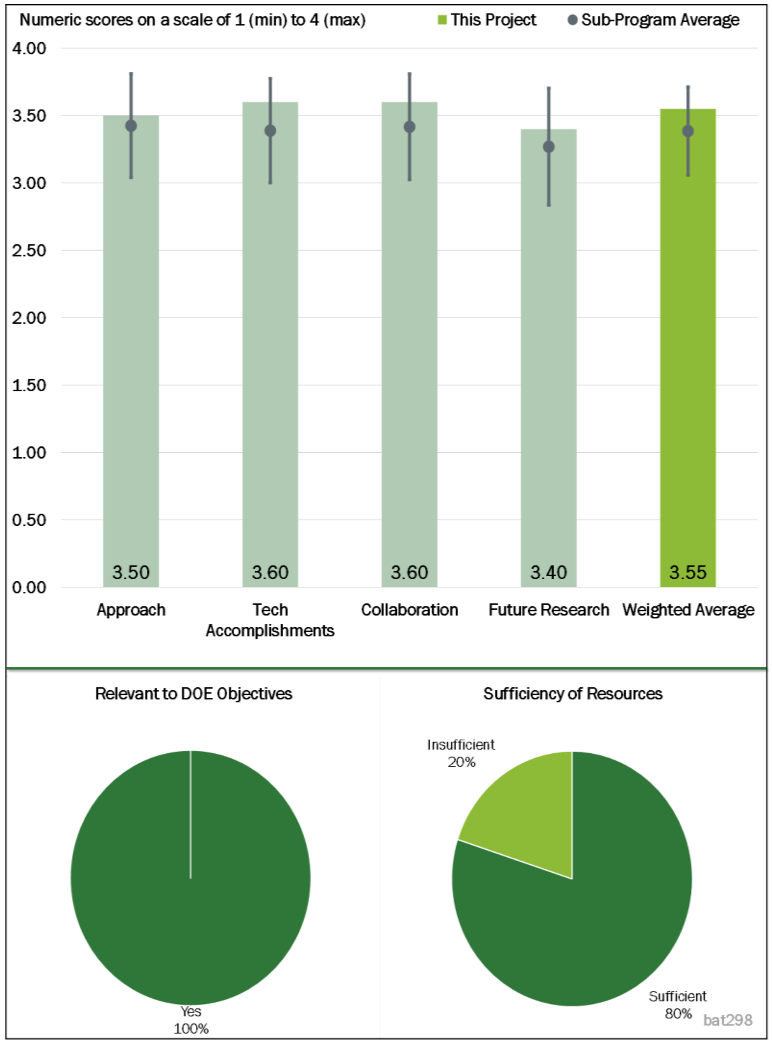

Figure 2-27 -Presentation Number: bat298 Presentation Title: Efficient Simulation and Abuse Modeling of Mechanical-Electrochemical-Thermal Phenomena in Lithium-Ion Batteries Principal Investigator: Shriram Santhanagopalan (National Renewable Energy Laboratory)

Presenter

Shriram Santhanagopalan, National Renewable Energy 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 and well-planned.

Reviewer 1:

The reviewer stated that this project has a well thought-out set of steps and tasks to combine the electrochemical modeling with mechanical-abuse modeling. The layout of the milestones and collaboration between the national laboratories should also contribute to the success of the project.

Reviewer 2:

Gap between the modeling tools and cell design is very well captured in this development tool, according to the reviewer. Collaborating with the right partners in both academia and industry expedites the development process and addresses the technical barriers.

Reviewer 3:

The reviewer commented that the project is well-designed. This is a good approach to develop effective simulation tools for practical assessment of battery safety and close the gap between materials R&D and modeling tools. The failure mechanism is also investigated in this project and guides the battery design.

Reviewer 4:

The approach seemed okay, but the reviewer was not sure what the PI meant by “efficient model.” The reviewer had some concern with the strain-rate and heat-transfer measurements. The reviewer noticed that the team has an ANSYS model image and LS- DYNA images. The images should be able to solve everything, including heat transfer (HT) in LS-DYNA.

Reviewer 5:

The reviewer commented that, having reviewed last year, the work is outstanding in nature with a few top-class people in the world. The reviewer felt that project may be a little behind schedule due to previous budget issues; the team should be given the opportunity to complete the project, and if the budget is available, the project should be allowed to continue on extension/proposed research for the next few years.

Regarding the reviewer's concern about beta-version commercialization and expected outcome, the presenters mentioned that one of the automobile companies has licensed the technology. Regarding the reviewer's concern about $80/kWh, the presenters think it will be possible with a thick electrode. Milestone 2.4 has been delayed. Argonne provided the experimental matrix data source. The reviewer suggested that in the design of experiments, the Taguchi fractional factorial design, the project team needs to decide which factors (porosity, thickness, diffusivity) and levels of experiments need to be repeated to reduce time.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

With very good understanding of the underlying issues and collaborating with the right technical partners, the reviewer noted that the researchers have accomplished the technical challenges. Cell testing and validating with the software tools is a nice development approach.

Reviewer 2:

According to the reviewer, some accomplishments have been demonstrated with publications in journals.

Reviewer 3:

The reviewer commented that the project appears to be making good progress towards the goals. The model-to-experimental data comparison for the computational efficiency portion of the project is impressive. The reviewer stated that it is harder to characterize the effectiveness of the Task 2 work because it is more difficult to compare experimental data to modeling data in the case of the mechanical modeling.

Reviewer 4:

The reviewer asserted that excellent progress has been made in the project. The project calibrated a Newman model to show the agreement of a macro-homogeneous model against the entire Cell Analysis, Modeling, and Prototyping (CAMP) Facility library. The mechanical-electrochemical-thermal model was developed for mechanical abuse simulation. All of these are good for mechanical characterization of cell components and the investigation of the complex failure mechanism. However, the identification and simulation in the project are based on Gr/NCM532. The reviewer wanted to know if the model is suitable for other battery systems, and how does it give a guide to designing new battery materials.

Reviewer 5:

The reviewer commented that, having reviewed last year, the work is outstanding in nature with a few top-class people in the world. The reviewer believed that the project may be a little behind schedule due to previous budget issues; the team should be given the opportunity to complete the project, and if the budget is available, the project should be allowed to continue on extension/proposed research for the next few years.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that the collaboration of academic researchers, industry partners, and DOE national laboratories has strengthened the development process. Integrating the development with software vendors adds significant value to the user community.

Reviewer 2:

The reviewer noted that this project contains many collaborators and partners. All the partners participate and contribute to the work of the project. The whole team is well coordinated and has a clear-cut division of labor.

Reviewer 3:

The collaboration seemed good to the reviewer, who suggested better collaboration and discussion about the high strain-rate data and discussions with the current collaborators at Ohio State University and George Mason University.

Reviewer 4:

It was clear to the reviewer there is good collaboration and coordination among the many laboratories on this project. The reviewer thought that the project could benefit from some industry partners to help focus the deliverables on the coupled mechanical modeling in Task 2.

Reviewer 5:

The reviewer commented that, having reviewed last year, the work is outstanding in nature with a few top-class people in the world. The reviewer perceived that project may be a little behind schedule due to previous budget issues; the team should be given the opportunity to complete the project, and if the budget is available, the project should be allowed to continue on extension/proposed research for the next few years.

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

Reviewer 1:

The reviewer stated that fracture of electrode composite is a complex problem and requires a very high level of understanding from many aspects. Researchers have proposed a well-thought out plan to capture these issues. Overall, the proposed future research is very good.

Reviewer 2:

In terms of future work, the reviewer commented that the project plan to use dynamic loading tests to characterize failure at higher strain rates is more reasonable than static testing.

Reviewer 3:

The reviewer said that if the budget is available, the project should be allowed to continue on extension/proposed research for the next few years on fracture experiments.

Reviewer 4:

The reviewer remarked that the progress on the project is impressive so far, with work done towards understanding the fundamentals of the mechanical abuse. It was harder for the reviewer to see how this can be used in a practical situation. Part of the focus of the future work should be on the applicability of the work on the design of battery packs.

Reviewer 5:

Future work seemed okay to this reviewer, who suggested that the PI get a little more organized because of the several important tasks going on here. The reviewer saw heat-transfer and strain-rate effects as the two important topics for future work. There probably needs to be some better discussion among collaborators. The heat-transfer model needs a little more work. It looks like there is a boundary-condition issue based on the plot provided on Slide 23. The reviewer also proposed that the PI consider interface conductance and assumed that the PI is modeling each of the layers as perfect conductors. The PI also needs to be careful with thermal-conductivity values used in the model as the reviewer wanted to know the source of these values, which should be temperature dependent. The reviewer asked about endo- and exothermic reactions contributing to heat transfer and whether these effects have been considered or whether the PI has been looking at thermal conductivity from the outside conducting through the stack. The reviewer added that the PI should set up some quick experiments to determine the thermal conductivity of each of the materials by themselves and then the bilayer conduction.

Other suggestions from the reviewer included taking a good look at, and holding discussions with, the collaborators about the strain-rate measurements shown on Slide 18. The reviewer expected that as the strain rate increases, the strain-to-failure (displacement) rate would decrease, and the reviewer also suggested that the strength-out rate would increase. If the PI is confident the results are correct, then there might be a contact effect that is causing increased displacement with increased strain rate. The reviewer recommended simulating this interaction with LS-DYNA to confirm this claim. The PI should also seek a discussion with some experts at SNL about strain-rate effects. There are researchers at SNL and Lawrence Livermore National Laboratory who do these strain rate effects (Split-Hopkins) measurements everyday. Also, the reviewer stressed looking into their technical reports for strain-rate experimental data as they have run a bunch of materials already that might be able to be used directly in the LS-DYNA models.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer observed that the project standardizes identification of the model parameters, increases computational efficiency, extends the models to include mechanical failure of cells and packaging components, and closes gaps between materials R&D and computer-aided engineering of batteries (CAEBAT) modeling tools. When the battery community uses these tools, the number and duration of battery test and module/pack costs can be significantly reduced. Thus, the project supports the overall DOE objectives.

Reviewer 2:

The reviewer responded affirmatively that this project should help with improving safety and lowering the development costs of vehicle batteries.

Reviewer 3:

The reviewer believed that DOE is trying to reduce the battery cost to $80/kWh and this kind of technically competent researchers can achieve DOE goal.

Reviewer 4:

The reviewer found the project to have great relevance.

Reviewer 5:

While the overall DOE objectives have been met and the relevance, barriers, and project plan are all good, the reviewer recommended that the researchers should consider highlighting what the main objective is.

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

Reviewer 1:

The reviewer thought that the project should get more funding to conduct mechanical-abuse testing of cells and modules and to help with the correlation between experiments and modeling on a cell or even module level.

Reviewer 2:

According to the reviewer, the team has experienced researchers and partners and is well-equipped with the necessary instruments that could allow the team to achieve the stated milestones in a timely fashion.

Reviewer 3:

The reviewer noted that the researchers have sufficient resources available to carry the task in a timely fashion and they have also documented that very well.

Reviewer 4:

Resources seemed good to the reviewer, who suggested trying to get some advice from an engineer at SNL on strain-rate effects on materials, contact surface, etc.

Reviewer 5:

While talking with presenters, the reviewer found that the DOE budget was a little bit of an issue so the project is behind schedule. The reviewer thought that in terms of knowledge or national laboratory resources, it is not a concern.

Presentation Number: bat299
Presentation Title: Microstructure Characterization and Modeling for Improved Electrode Design
Principal Investigator: Kandler Smith (National Renewable Energy Laboratory)

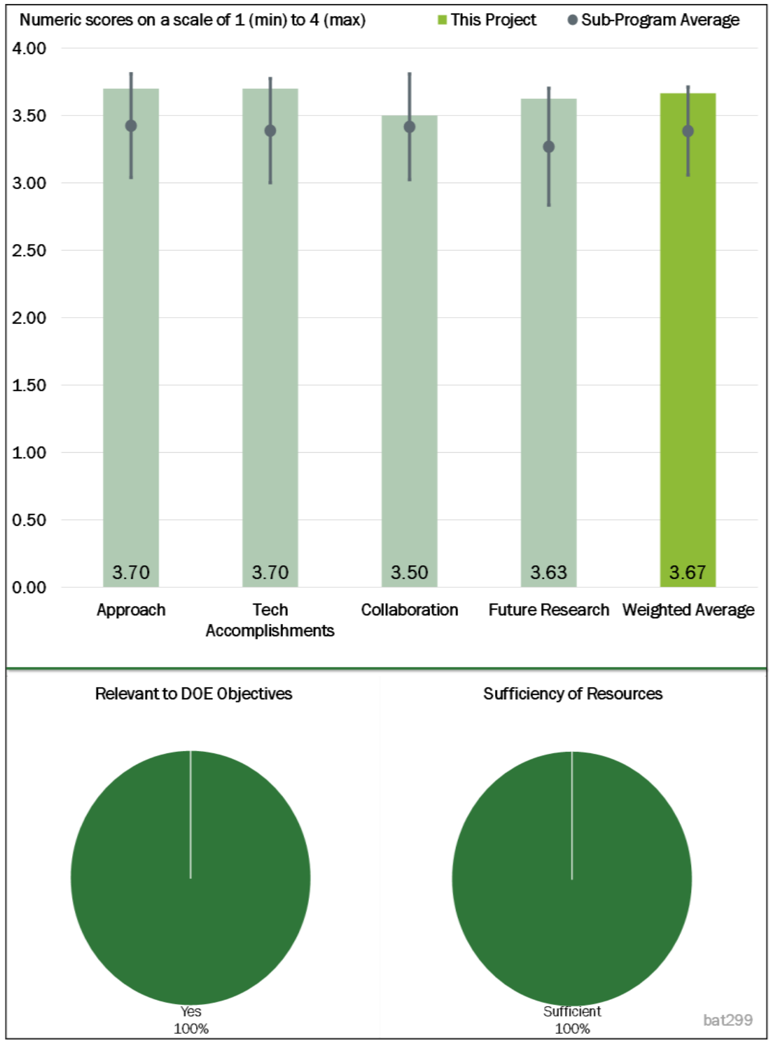

Figure 2-28 - Presentation Number: bat299 Presentation Title: Microstructure Characterization and Modeling for Improved Electrode Design Principal Investigator: Kandler Smith (National Renewable Energy Laboratory)

Presenter

Kandler Smith, National Renewable Energy 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 and well-planned.

Reviewer 1:

The approach seemed great to the reviewer, and it looked as if the project team is getting some good information from the model.

Reviewer 2:

Overall, the reviewer remarked that this is a very interesting project addressing a gap in the currently available battery modeling tools. The approach towards the technical challenges is well thought-out and the project is showing results.

Reviewer 3:

The reviewer commented that the researchers addressed the technical barrier in microstructure characterization sufficiently. Electrode design through mesoscale modeling is well designed and feasible.

Reviewer 4:

The reviewer commented that, having reviewed last year, the work is outstanding in nature with a few top-class people in the world. The reviewer believed that project may be a little behind schedule due to previous budget issues; the team should be given the opportunity to complete the project, and if the budget is available, the project should be allowed to continue on extension/proposed research next few years.

Regarding the reviewer’s concern about beta-version commercialization and expected outcome, the presenter mentioned that one of the automobile companies has licensed the technology. Regarding the reviewer’s concern about \$80/kWh, the presenters think it will be possible with a thick electrode. Milestones 2.3 and 2.4 appear to be new as they were not there in 2017. Argonne provided the experimental matrix data source on Slide 15. The reviewer suggested that in the design of experiments, the Taguchi fractional factorial design, the project team needs to decide which factors (porosity, thickness, diffusivity) and levels of experiments need repeating to reduce time. In discussions with the presenter about the binder for the model on Slide 9, the reviewer learned that polyvinylidene difluoride (PDVF) and the Purdue University model were used. The reviewer recommended that be used in future presentations. The reviewer also suggested that the presenter use impedance instead of resistance with a C-rate plot although the reviewer wad told that the nature of the plot would not change. In discussing the 1C and 5C rates on Slide 12, the reviewer learned that the maximum is 12C and the presenters are aware of that. Lastly, the reviewer mentioned the team finally discussed the remaining challenges and barriers.

Reviewer 5:

The reviewer pointed out that the developed microstructure modeling and characterization well-predicted the impact of the electrode recipe and design on electrode performance at different C rates and electrode thicknesses. However, some problems need to be considered during the modeling analysis to further shrink the gaps between the modeling and practical cell design. First, because the resistance changes with increasing electrode thickness, the effects of electrode thickness on microstructural-resistance analysis and rate capability need to be considered. Second, the resistance analysis at different cycle life should be considered because the internal resistance will change during cycling. Finally, the anode side needs to be considered during the modeling or resistance analysis because the Gr electrode would probably bear the similar microstructural problems.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer pronounced the accomplishments to be great.

Reviewer 2:

The reviewer stated that there are still there are many challenges in mesoscale modeling of electrodes. The authors attempted to address all the challenges through imaging, simulation, and homogenization to achieve desired performance indicators.

Reviewer 3:

The reviewer found the technical accomplishments for this project to be very interesting and looked forward to seeing the results of the final phase of the project.

Reviewer 4:

The developed microstructure modeling and characterization has made great progress toward overcoming the barriers and conforming to the schedule, according to the reviewer. The effects of the electrode recipe and morphologies (e.g., electrode thickness, tortuosity due to C-binder, porosities, particle size or shape) on electrode performance have been well modeled and validated by experiments. However, for better predicting or instructing the industrial cell design, more efforts need to be made, like fulfilling the model by considering more comprehensive factors (e.g., cycling life, temperature, etc.) and validating from more battery-cycling experiments (e.g. long-term cycling, different loading, and C rate).

Reviewer 5:

The reviewer commented that, having reviewed last year, the work is outstanding in nature with a few top-class people in the world. The reviewer believed that project may be little behind schedule due to previous budget issues; the team should be given the opportunity to complete the project, and if the budget is available, the project should be allowed to continue on extension/proposed research next few years.

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Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
It looked to the reviewer as if the collaborators are working well together.

Reviewer 2:
The reviewer stated that the collaboration was outstanding, and Kander is handling it very well.

Reviewer 3:
The reviewer commented that there were good collaborations with various partners from national laboratories to universities. All the partners with their distinct advantages participate and are well coordinated to contribute to the progress of the project.

Reviewer 4:
The reviewer remarked that the project was well coordinated among DOE national laboratories and academia. The addition of an industry partner will help to identify the real time and practical risks.

Reviewer 5:
The reviewer stated that this project and the other related projects are successfully working within the national laboratory and university system. The reviewer thought that the project would benefit from industry partners to help with the practical application of the work being done.

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

Reviewer 1:
The reviewer commented that design inputs, validation, and performance against multiple design are logical steps considering the technical barriers and effective realization of the technology. Particle approach, electrode mechanics, and application of design studies for new materials address alternating development paths and attempts to mitigate risks.

Reviewer 2:
The reviewer suggested looking at temperature-dependent materials models and how they might be implemented. Other ideas for consideration are including advection of the electrolyte in addition to diffusion, and validating conductivity predictions. The reviewer was not sure if changes in conductivity as a function of temperature had been considered. The localized conductivity will decrease with increase in temperature.

Reviewer 3:
The reviewed viewed the future work as exactly right for this project. One big challenge will be to obtain the 3-D views of the carbon + binder domain (CDB). This would be particularly helpful in the design of fast-charge anodes for high energy-density EV cells.

Reviewer 4:
The reviewer stated that if the budget is available, the project should be allowed to continue on extension/proposed research for the next few years.

Reviewer 5:
The reviewer said not applicable.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
Through the systematic microstructure modeling and characterization, the reviewer noted that some key factors that affect the electrode performance can be screened out and some fundamental understanding of the electrode design could be provided. These factors can be used to guide practical electrode fabrication for further improving battery performances or enhancing the energy densities. Therefore, this project supports the overall DOE objectives. The reviewer said that the project captures the overall DOE objectives. Microstructure imaging of carbon-binder domain (CBD) at different cycles to capture the randomized particle sizes will be helpful for stochastic evaluation.

Reviewer 2:
The reviewer affirmatively found the project to be very relevant. This project turned out really well, and the reviewer thought that others can really build off these findings.

Reviewer 3:
The reviewer responded yes, and noted that battery-cost reduction to make EVs practical and setting a goal of $80/kWh are right in target.

Reviewer 4:
The reviewer stated that the project captured the overall DOE objectives.

Reviewer 5:
The reviewer affirmatively commented that this and the other CAEBAT modeling projects do support the DOE goals to reduce the cost of battery development. The reviewer noted that these projects would greatly benefit from an industry partner to make sure they can be used as intended by Li-ion battery cell designers to lower the development costs.

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

Reviewer 1:
The resources seemed sufficient to the reviewer to support the current level of research.

Reviewer 2:
Resources are sufficient for this project, according to the reviewer.

Reviewer 3:
The reviewer said the resources were good.

Reviewer 4:
The reviewer thought that the resources are appropriate for this program, but more resources may be needed for the 3-D imaging of the CBD.

Reviewer 5:

The reviewer felt that project may be a little behind schedule due to previous budget issues; the team should be given the opportunity to complete the project, and if the budget is available, the project should be allowed to continue on extension/proposed research for the next few years.

Presentation Number: bat300
Presentation Title: Enhancement and Deployment of VIBE, the Open Architecture Software (OAS) Environment
Principal Investigator: Srikanth Allu (Oak Ridge National Laboratory)

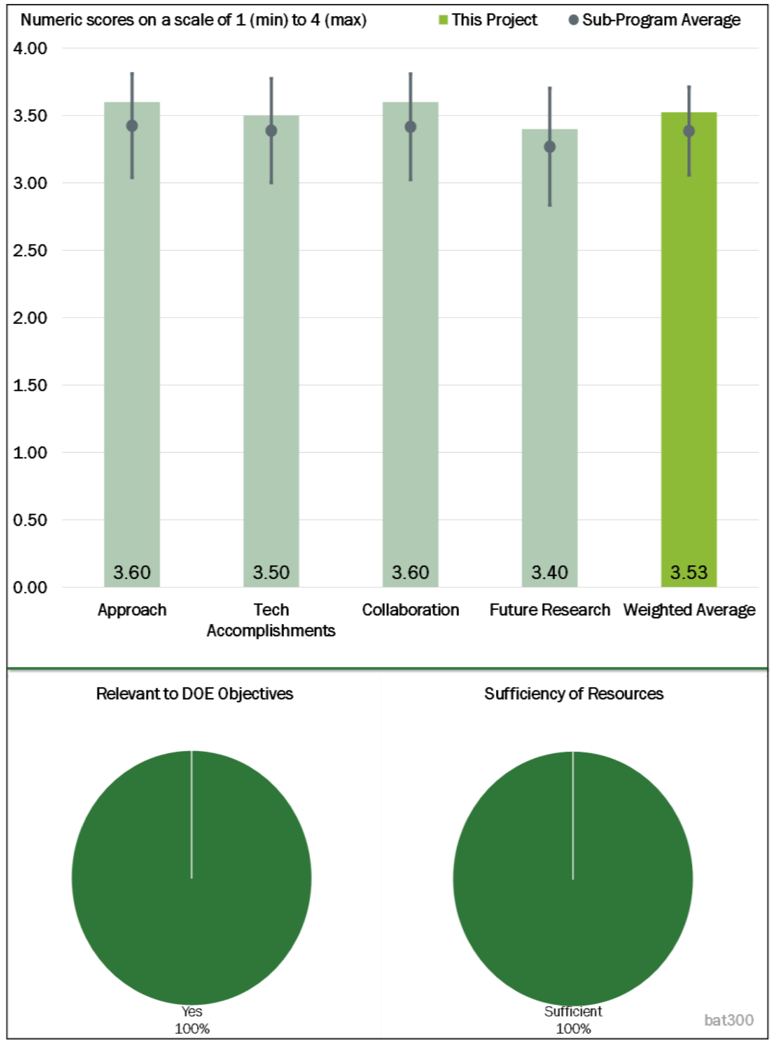

Figure 2-29 - Presentation Number: bat300 Presentation Title: Enhancement and Deployment of VIBE, the Open Architecture Software (OAS) Environment Principal Investigator: Srikanth Allu (Oak Ridge National Laboratory)

Presenter

Srikanth Allu, Oak Ridge 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 and well-planned.

Reviewer 1:

The reviewer remarked that this project helps design a tool to allow researchers to explore battery response under both normal and abusive conditions. The simulation and experimental results show us what is happening when a Li-ion battery gets a short circuit, it is helpful to design battery management systems for safe operation of large battery packs.

Reviewer 2:

The reviewer stated that the approach is excellent.

Reviewer 3:

The reviewer said that major barriers of battery energy density are addressed very well from the perspectives of physical phenomena as well as predictive simulation tools.

Reviewer 4:

Overall, the reviewer commented that this is a very interesting project that addresses a gap in the currently available battery modeling/simulation tools.

Reviewer 5:

The reviewer noted that the approach seems fine, but wanted to have seen more validation if possible.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that the experimental and simulation results show us what is happing when a Li-ion battery gets a short circuit: separator failure criterion, microstructure reorganization under mechanical loading, and fragmentation of anode-current collectors.

Reviewer 2:

By developing new experiments, capturing fragmentation of anodes, and reconstructing the fragmentation problems, the reviewer stated that the technical accomplishments are augmented. Accomplishments are correlated well against the measured performed indicators.

Reviewer 3:

For section 1.4 in the poster, the reviewer noted that the demonstrated ability to predict the onset of a short from mechanical deformation was not present, so it is very difficult to determine if this statement is true or not. Most of the conclusions on Slide 10 were given without data to back up the claims.

Reviewer 4:

The reviewer reported that the PI mentioned that the project is 75% complete although the poster says 55%. The PI mentioned to the reviewer that due to budget constraints there may be a possibility of project delay.

Reviewer 5:

The reviewer wanted more validation of the model with experiments.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that the collaboration with national laboratories (SNL, LBNL, ANL, and National Renewable Energy Laboratory [NREL]) can not only provide some experimental results and advanced techniques to this project, but also they can help analyze whether the designed simulation method is correct or not.

Reviewer 2:

The Involvement of different DOE national laboratories adds more value to the project, according to the reviewer.

Reviewer 3:

The reviewer observed excellent collaboration, and reported having mentioned to the PI work between ORNL and the DOT that was not mentioned in reference to *Crashworthiness Models for Automotive Batteries, A Report on the Department of Energy Project 2088-A031-15 for the National Highway Traffic Safety Administration (NHTSA), an Agency of the U.S. Department of Transportation* (J. A. Turner, S. Allu, et al. 2018), which discusses fragmentation of copper anode, etc..

Reviewer 4:

Collaboration seemed good to the reviewer, who suggested trying to find a point of contact at Nissan to collaborate with in order to get more information about Leaf battery testing. That would yield potentially more data to validate against.

Reviewer 5:

The reviewer asserted that this project and the other related projects are successfully working within the national laboratory and university systems. The reviewer thought that the project would benefit from industry partners to help with the practical application of the work being done.

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

Reviewer 1:
The reviewer stated that the project aims to develop a tool to allow researchers to explore battery response under both normal and abusive conditions. However, when the battery gets a short, lots of things will happen within a short time. Thus, it is pretty challenging to simulate what is happening on a battery short circuit. The future research plan comes up with some other methods for further study and understanding battery response.

Reviewer 2:
According to the reviewer, researchers have considered broad areas to address for future research. High-computation risk mitigation using reduced-order modeling and integration of different models to provide alternating development avenues are interesting approaches.

Reviewer 3:
The reviewer wanted to see an experimental approach included that demonstrates this model's ability to truly detect an onset of a short-based on-mechanical deformation.

Reviewer 4:
The reviewer stated that some of the remaining challenges and barriers mentioned by the PI should be allowed to continue, e.g., insufficient understanding of thermal runaway and internal shorts due to Li plating.

Reviewer 5:
The reviewer wanted more validation of the model.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer remarked that this project supports the overall DOE objectives to develop a Li-ion battery with higher energy density, which requires much more strict control on battery safety. This project uses the simulation tool to understand battery response under both normal and abusive conditions, which is helpful to design battery management systems.

Reviewer 2:
The reviewer stated that the project addresses the overall DOE objectives. Simulation gaps and underlying insufficiencies in physical phenomena are identified and addressed properly

Reviewer 3:
There is understanding of the physical phenomena for battery safety and performance, according to the reviewer.

Reviewer 4:
The reviewer found great relevance.

Reviewer 5:
The reviewer responded affirmatively and elaborated that this and the other CAEBAT modeling projects do support the DOE goals to reduce the cost of battery development. The reviewer thought that these projects would greatly benefit from an industry partner to make sure they can be used as intended by Li-ion battery cell designers to lower the development costs.

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 the team and its collaborators have sufficient resources to go on with the research and achieve the stated milestones, including designing new experiments, advanced characterization techniques, and powerful simulation tools.

Reviewer 2:

The reviewer said that sufficient resources are available for researchers to pursue this project.

Reviewer 3:

The reviewer commented that resources are appropriate for the project.

Reviewer 4:

The reviewer stated that the overall project has the support of the best technical resources; if the budget is not a constraint, then the project can be completed on time.

Reviewer 5:

Resources seem good to the reviewer, who noted that, actually, there are a lot of people working on this project. The reviewer expected some more claims coming from this work and suggested that the PI evaluate everyone's contribution and make sure everyone is contributing who is being paid on this project.

Presentation Number: bat301
Presentation Title: Experiments and Models for the Mechanical Behavior of Battery Materials
Principal Investigator: Sergiy Kalnaus (Oak Ridge National Laboratory)

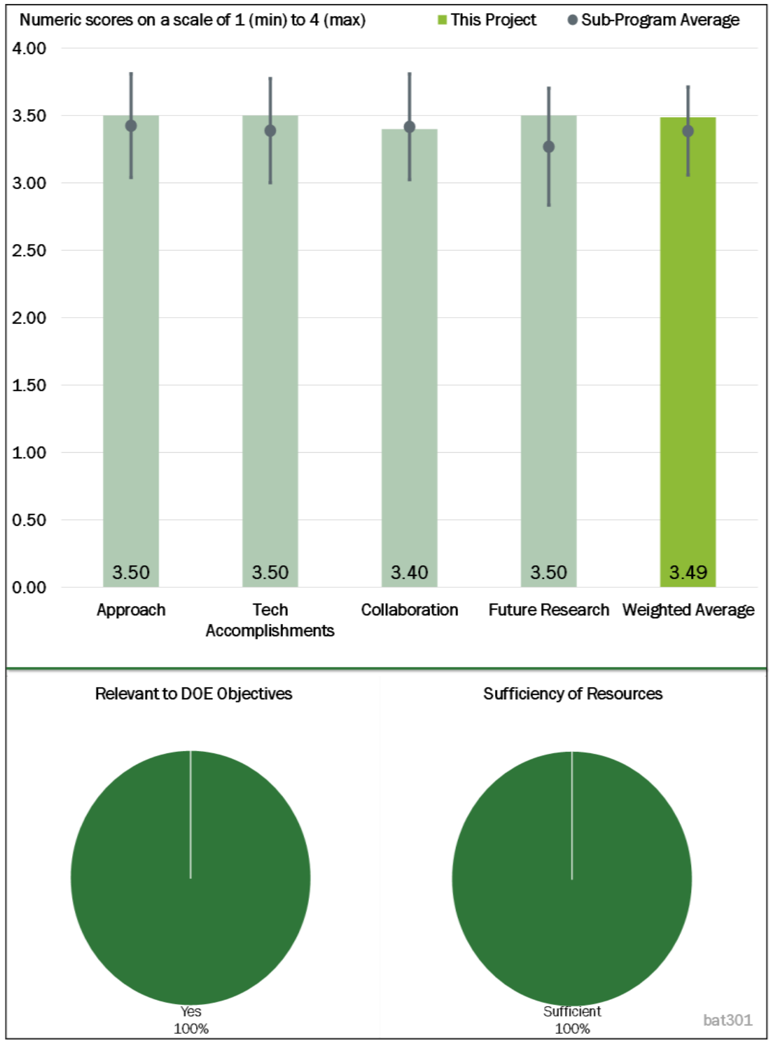

Figure 2-30 - Presentation Number: bat301 Presentation Title: Experiments and Models for the Mechanical Behavior of Battery Materials Principal Investigator: Sergiy Kalnaus (Oak Ridge National Laboratory)

Presenter

Sergiy Kalnaus, Oak Ridge 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 and well-planned.

Reviewer 1:

The reviewer noted that, generally speaking, the approach that the ORNL group has adopted is well designed and feasible. It is effective to develop mechanics models and failure criteria based on measurements of mechanical properties and other models (E-Chem, thermal). The methods that the group chose for investigation, like biaxial deformation test and X-ray tomography tests, are efficient to investigate failure criteria and address technical barriers.

Reviewer 2:

Overall, the reviewer stated that this is a very interesting project addressing a gap in the currently available battery-modeling tools. The approach towards the technical challenges is well thought-out and the results demonstrate that.

Reviewer 3:

According to the reviewer, researchers have a well-defined approach to addressing the technical barriers and relevance. Coordinating experimental and simulation work in parallel is a good plan.

Reviewer 4:

The reviewer liked the approach, and there is some good information here that others could use.

Reviewer 5:

The reviewer said that the project is feasible and well designed, and the team has addressed the technical barrier.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that mechanical properties of the cell components are being measured, and researchers have a thorough understanding of the complex behavior of each component. The project team has made an excellent effort to understand the conditions for short circuits.

Reviewer 2:

The reviewer noted that this is a very important part of the modeling work, and it would be interesting to see the effects of cell aging on the properties in this study.

Reviewer 3:

The reviewer pointed out that the digital image correlation (DIC) measurements look consistent with failure. However, the reviewer expected a strain field more like the model is showing and posited that there must be a bias in the experiment. The reviewer asked if the sphere is perfectly in the center.

The reviewer said the PI might also consider whether to add the holes into the finite element analysis simulation. This approach would allow using a shell element to model the voids and run the mesh cells upwards of 1 million cells to reach a more realistic simulation. According to the reviewer, the cracking on the current collector looks like an adhesion failure between the layers, as if the materials are actually adhering to the neighboring layer and failing when the layers relax after loading.

Reviewer 4:

The reviewer mentioned that the project is 75% complete, and it appears that a 1-year extension will help to complete it. The project is a little behind schedule on some milestones (e.g., I.5, C.3, C.4, C.5, C.6, I.6) because of budget constraints as mentioned by the PI.

Reviewer 5:

The progress of the project is generally effective, according to the reviewer. However, there is still 25% percent of the project needs to be completed so far as mesoscale simulations, deployment of virtual integrated battery environment/open architecture software (VIBE/OAS) with the integrated multiscale capability, and other milestones that have not been reached yet.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found good collaboration with DOE national laboratories. Including the CAEBAT project team helps to speed up the development process cross functionally.

Reviewer 2:

The reviewer observed excellent collaboration, and reported having mentioned to the PI work between ORNL and DOT that was not mentioned in reference to *Crashworthiness Models for Automotive Batteries, A Report on the Department of Energy Project 2088-A031-15 for the National Highway Traffic Safety Administration (NHTSA), an Agency of the U.S. Department of Transportation* (J.A. Turner, S. Allu et al. 2018), which discusses fragmentation of copper anode, etc.

Reviewer 3:

This project has good collaboration with its project team, according to the reviewer.

Reviewer 4:

The reviewer said that the collaboration was good.

Reviewer 5:

The reviewer observed that the partners in the project team are well coordinated and have made their own contribution to the overall project. However, SNL did not complete milestone C.3 on time, and the contribution of ANL is unclear.

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 asserted that researchers have identified critical areas for future research both experimentally as well as simulation.

Reviewer 2:

Biaxial testing of electrodes sounded good to the reviewer.

Reviewer 3:

The reviewer stated that the future work is well thought-out. The reviewer was glad to see the effects of aged components included because the mechanical properties could change with cycling/exposure to the electrolyte.

Reviewer 4:

The reviewer noted that the PI had mentioned that proposed future research is ongoing, e.g., biaxial compression of electrodes, in situ X-ray tomography.

Reviewer 5:

According to the reviewer, the proposed future research plan has included the key points that should be accomplished in the future although more details of the plan could be given.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

This project supports the overall DOE objectives, according to the reviewer. This project has investigated the physical phenomena in batteries and proposed mechanics models and failure criteria. All of these research results are beneficial for increasing battery performance.

Reviewer 2:

The reviewer noted that this better understanding of failure of battery-electrode materials will help with battery safety.

Reviewer 3:

The reviewer commented that, overall, the project addresses the DOE objectives.

Reviewer 4:

The reviewer responded affirmatively and said that the work was relevant.

Reviewer 5:

The reviewer affirmed that this and the other CAEBAT modeling projects do support the DOE goals to reduce the cost of battery development. The reviewer thought that these projects would greatly benefit from an industry partner to make sure they can be used as intended by Li-ion battery-cell designers to lower the development costs.

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 there sufficient resources have been allocated to perform the task.

Reviewer 2:

The reviewer commented that resources are appropriate for the project.

Reviewer 3:

The reviewer noted that the project is a little behind schedule at 75% complete, which the PI mentioned was mainly due to budget issues at the beginning of the fiscal year. It seemed to the reviewer that the team will be able to complete another year.

Reviewer 4:

The project has sufficiently used the resources for the project to achieve the stated milestones, although the team has not yet reached some of the milestones.

Reviewer 5:

The reviewer suggested looking at the sand models from LS-DYNA as they may help with granular modeling and validation.

Presentation Number: bat302
Presentation Title: Microstructure Imaging and Electrolyte Transport Property Measurements for Mathematical Modeling
Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

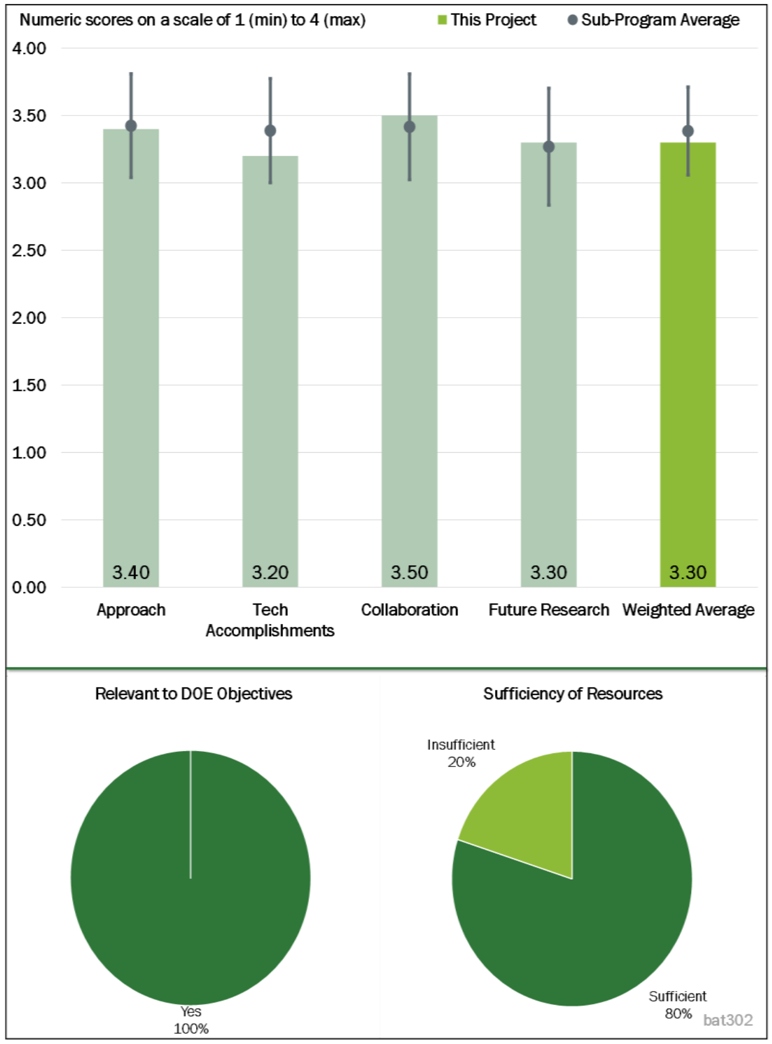

Figure 2-31 - Presentation Number: bat302 Presentation Title: Microstructure Imaging and Electrolyte Transport Property Measurements for Mathematical Modeling Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

Presenter

Venkat Srinivasan, 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 and well-planned.

Reviewer 1:

The reviewer stated that this project aims to provide electrochemical properties, such as ionic diffusivity and conductivity, as input data for a multiphysics simulation tool developed in another project. In addition, a correlation between electrode thickness and SOC was achieved in initial cycles with slow charging. The project is well-designed.

Reviewer 2:

The reviewer commented that this is a very interesting project, well designed, and an important piece of information to feed into the modeling project.

Reviewer 3:

The reviewer remarked that the approach that was used is fairly effective. The collection of in-operando images using cycled electrode materials is important to support modeling results.

Reviewer 4:

The reviewer found that the researchers had made good progress in capturing the relevant images of electrodes. Overall, the reviewer found this to be a well-defined approach.

Reviewer 5:

The approach seemed okay to the reviewer, and this is a necessary task to determine the internal structure. However, the reviewer was not sure the beam-line source is the best method. There are several industrial and medical computerized tomography (CT) machines that will provide equivalent resolution. All the reconstruction algorithms have been developed. Actually, there has been extensive research on frequency-domain methods that filter and reconstruct the volumes. The reviewer was not sure that CD-adapco really has the momentum to beat many of these established methods. Something more interesting about these industrial and medical CT machines is that transient information can be captured, which means that the battery can be charged and discharged while capturing the CT information. This is commonly done to look at the fluid flow through porous media. So, the reviewer was not convinced that the beam-line source is the best option. What would be interesting would be doing a neutron-imaging technique to get a better grasp on the C formation, such as a neutron spallation experiment with the beam line. This technique is actually used to see atomic hydrogen and oxygen so there should not be a problem seeing atomic C. The reviewer pointed out that this technique has been employed to look at crack propagation in superalloys.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer stated that most of the tasks have been accomplished and the milestones have been reached. Necessary results have been collected by collecting in-operando images.

Reviewer 2:

The reviewer found the technical accomplishments and progress towards overall project to be good. The team obtained electrode image data from cycled electrode material and a developed post-processing pipeline for tomographic reconstructions of cycled electrodes.

Reviewer 3:

Accomplishments seemed good to the reviewer. The team was able to capture the thickness, which is useful information. The reviewer wanted to see the team do a CT scan during transient operation. The reviewer also wanted the team to consider a technique that can capture information about the C.

Reviewer 4:

The reviewer said that the findings of this project were very interesting/surprising. If possible, the cathode expansion study should be tried on a few different electrode designs to see if the results are the same. It would also be interesting to apply the technique to aged cells and anode materials.

Reviewer 5:

The reviewer indicated the project needs more performance indicators and relevant data to augment the quantitative imaging correlation. Simulation needs more quantifiable data points in addition to microstructure imaging.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that the project team collaboration for the modeling project is very good and utilizes the strengths of the national laboratory system.

Reviewer 2:

The reviewer asserted that the partners on the team participated fully in the project. Each member has made a significant contribution to the project.

Reviewer 3:

The reviewer said the partners participated actively and are well coordinated.

Reviewer 4:

The reviewer found good collaboration with different DOE national laboratories. The addition of industry partner and academia will bring more ideas and viewpoints.

Reviewer 5:

The reviewer indicated that there was good collaboration with the beam source and encouraged keeping this collaboration going; however, the reviewer suggested looking at how to use the neutron spallation source. The reviewer would have had CD-adapco focus on developing a DIC-type method that can be used with the transient CT information. This would allow predictions of internal strains within the battery. The reviewer warned against having CD-adapco waste time developing static CT-volume reconstruction. This has been developed already for the medical and industrial CT machines.

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

Reviewer 1:

The reviewer stated that the proposed future research is detailed, well-organized, and feasible.

Reviewer 2:

According to the reviewer, researchers identified and proposed effective research plans and addressed critical areas for improvement and opportunities.

Reviewer 3:

The reviewer said that the proposed future research is logical, including milestones and risk management.

Reviewer 4:

The reviewer mentioned that it is unfortunate that this project is ending. The technique has a lot of potential, and it should be developed further using a variety of samples.

Reviewer 5:

The reviewer indicated that the research seems to be going in the direction of transient CT reconstruction and capturing the CT information as the cell is running. However, the reviewer proposed doing this in an industrial or medical CT machine because these data can be captured pretty easily. Also, in these machines, the sample is static and not moving and that would address the issue of samples moving; these machines have solved this issue. The reviewer advocated for having CD-adapco work on the DIC method with transient CT information and looking into using the spallation source to resolve C material. These steps would help several of the other projects, including C, in their simulation.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer commented that this project supports the overall DOE objectives. This project collected and analyzed in-operando image data of the cycled electrode, which are significant and helpful for the modeling results and support of overall DOE objectives

Reviewer 2:

The reviewer said that the research encompasses all the DOE objectives. Low performance and high cost are the barriers, and the research aims to address these barriers.

Reviewer 3:

The reviewer remarked that this project supports the overall DOE objectives of providing accurate simulation-input data for CAEBAT teams, enabling construction of accurate models to guide cost and performance optimizations.

Reviewer 4:
The reviewer affirmed that the research is relevant to DOE goals.

Reviewer 5:
The reviewer responded affirmatively, and explained that this and the other CAEBAT modeling projects do support the DOE goals to reduce the cost of battery development. The reviewer thought that these projects would greatly benefit from an industry partner to make sure they can be used as intended by Li-ion battery cell designers to lower the development costs.

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 resources are sufficient and the stated milestones have been achieved in a timely fashion.

Reviewer 2:
There are sufficient resources allocated to carry out this research, according to the reviewer.

Reviewer 3:
The reviewer stated that the research team has sufficient funding, human resources, and equipment to complete the project.

Reviewer 4:
The reviewer noted that the funds are sufficient, but it would be good to see the project extended into the future.

Reviewer 5:
The reviewer suggested finding a medical or industrial CT machine. DOE National Energy Technology Laboratory has both machines and has run these reconstructions already. DOE Oak Ridge probably has these machines. The reviewer urged just look around within the DOE system as these machines are around. Also, the reviewer suggested getting time on the spallation source at the beam line.

Presentation Number: bat303
Presentation Title: Exploring How Electrode Structure Affects Electrode-Scale Properties Using 3-D Mesoscale Simulations
Principal Investigator: Scott Roberts (Sandia National Laboratories)

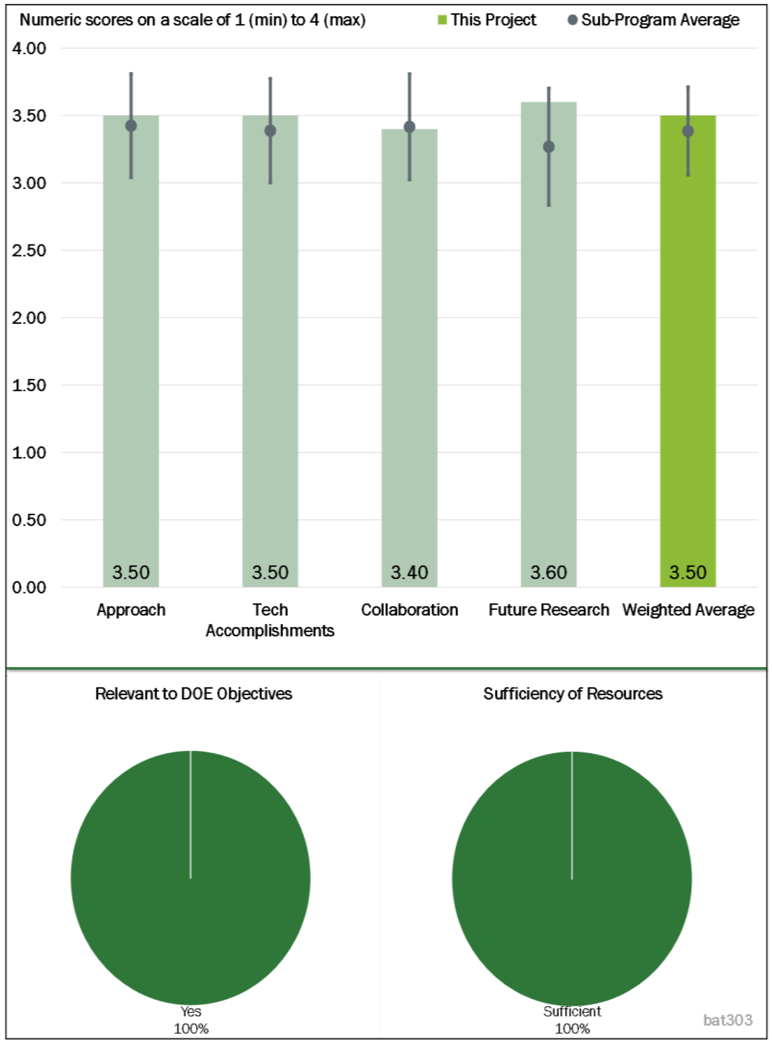

Figure 2-32 - Presentation Number: bat303 Presentation Title: Exploring How Electrode Structure Affects Electrode-Scale Properties Using 3-D Mesoscale Simulations Principal Investigator: Scott Roberts (Sandia National Laboratories)

Presenter

Scott Roberts, Sandia National Laboratories

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 and well-planned.

Reviewer 1:

The reviewer mentioned that the researcher used a different approach to address the technical barrier. The reviewer found the use of the discrete-element method (DEM) to be well designed and a feasible approach. This method allows the researcher to use many attributes of the electrode characteristics and provides a better understanding.

Reviewer 2:

In this project, the reviewer noted that a mesoscale model has been developed to perform coupled, mechanical-electrochemical discharge simulation of the battery. The nanoporosity in the CBD, for the first time, is being included in the mesoscale model.

Reviewer 3:

The reviewer said that, overall, the battery-modeling project is well designed to address the gaps in the current battery-modeling environment.

Reviewer 4:

The reviewer pronounced that approach as seeming good. This DEM method seems interesting and is a good method.

Reviewer 5:

The reviewer commented that the project objective is to understand the decaying behavior of batteries due to cycling through simulation of charging cathode material. To achieve this, the investigation was conducted to understand the effect of different components (i.e., CBD, binder, porosity, etc.) on the properties of the electrode. However, the lack of experimental validations of electrode response impedes the complete effectiveness of the approach.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer stated that the project has progressed well during the time duration proposed. The role of electrode parameters on the properties has been investigated pending experimental validation for final refined simulation.

Reviewer 2:

The reviewer said that the method to capture the images of the particles and mesh them at their micro-thickness level provides a good performance enhancement.

Reviewer 3:

The technical accomplishments and progress towards overall project are excellent, according to the reviewer. The team has demonstrated a robust and verified approach for three-phase cathode mesostructure representation and developed an understanding of the role of nanoporous CBD, how to construct them, and scale up the mesoscale results for use in macroscale (ORNL) battery abuse code.

The reviewer wanted to know the pixel and voxel resolution in the images, how the authors can make sure the connectivity of the solid phase is in order to perform continuum simulation, and how the authors can make sure no excessive micro/nanostructure has not been added. The reviewer also asked which machine learning segmentation algorithm was used and whether it was a supervised or unsupervised learning method.

Reviewer 4:

Accomplishments seemed good to the reviewer, who expressed a little concern with the electrical conductivity plot on Slide 12 because the reviewer did not expect the conductivity to be linear. The reviewer asked how the investigators are determining the material properties of the constitutive materials.

Reviewer 5:

The results were interesting to the reviewer, but it is hard to determine the accuracy of the modeling work without correlation with experimental data.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that there is excellent collaboration and engagement with relevant teams to speed up the development process.

Reviewer 2:

The reviewers said that the partners participated actively and are well coordinated.

Reviewer 3:

Collaboration seemed good to the reviewer, who suggested helping the collaborators that are imaging the C formation. The reviewer suggested having the collaborators run Raman spectroscopy to determine the sp2 sp3 content of the C. This will give a better idea of the electrical conductivity.

Reviewer 4:

According to the reviewer, the project team collaboration for the modeling project is very good and utilizes the strengths of the national laboratory system; however, for this project, one focus of the collaboration should be to provide validation data for the models through experimentation.

Reviewer 5:

The reviewer stated that the tasks seem organized and divided among the team collaborators. However, the distinction between LBNL and ANL contribution in tomography is not clear.

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

Reviewer 1:

The reviewer stated that the project has identified several points of risks and challenges and addressed them in the future work. Most notably, LBNL/ORNL will be providing experimental data to validate the simulation.

Reviewer 2:

The reviewer found the proposed research very sharply focused on delivering accurate responses. The researcher addressed the risks associated with the barriers and suitable risk-mitigation strategies.

Reviewer 3:

The reviewer said that the proposed future research is logical, including milestones and risk management.

Reviewer 4:

The future work planned for this project addresses the major gaps, according to the reviewer.

Reviewer 5:

The reviewer called the research good and urged continuing to work on the DEM method. Also, the reviewer suggested trying to get a better idea of the properties of the constitutive materials, the sp2 sp3 content of C.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer pointed out that the project is tightly related to DOE objectives because it addresses energy security and efficiency topics. It is understood that the outcome of this project could potentially limit the loss of energy and power in batteries used in vehicles by simulating and abusing cathode electrodes.

Reviewer 2:

The reviewer commented that the loss of power and energy and abuse tolerance, reliability, and ruggedness are the barriers and the DOE objective of improving the fidelity of battery-scale simulation fits the bill perfectly.

Reviewer 3:

The reviewer said that this project supports the overall DOE objectives by improving the fidelity of battery-scale simulations of abuse scenarios through the creation and application of microscale (particle-scale) electrode simulations

Reviewer 4:

The reviewer affirmed that the project was very relevant to DOE goals of improvements in battery technology.

Reviewer 5:

The reviewer responded affirmatively, and elaborated that this and the other CAEBAT modeling projects do support the DOE goals to reduce the cost of battery development. The reviewer thought that these projects would greatly benefit from an industry partner to make sure they can be used as intended by Li-ion battery cell designers to lower the development costs.

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

Reviewer 1:
The reviewed agreed that sufficient resources are available to the researcher to accomplish the project milestones in a timely fashion.

Reviewer 2:
The reviewer stated that the research team has sufficient funding, human resources, and equipment to complete the project.

Reviewer 3:
The reviewer stated that the funds are sufficient, but it would be good to see the project extended into the future.

Reviewer 4:
The resources seemed appropriate and sufficient to the reviewer. Large-scale simulation has been undertaken, and the lack of experimental validation due to unavailability of raw data for validation is the only missing link for the ongoing simulation.

Reviewer 5:
Resources seemed good to the reviewer, who wanted to see a couple of additional experimental methods to determine materials of constitutive materials.

Presentation Number: bat307
Presentation Title: Discovery of High-Energy Lithium-Ion Battery Materials
Principal Investigator: Wei Tong (Lawrence Berkeley National Laboratory)

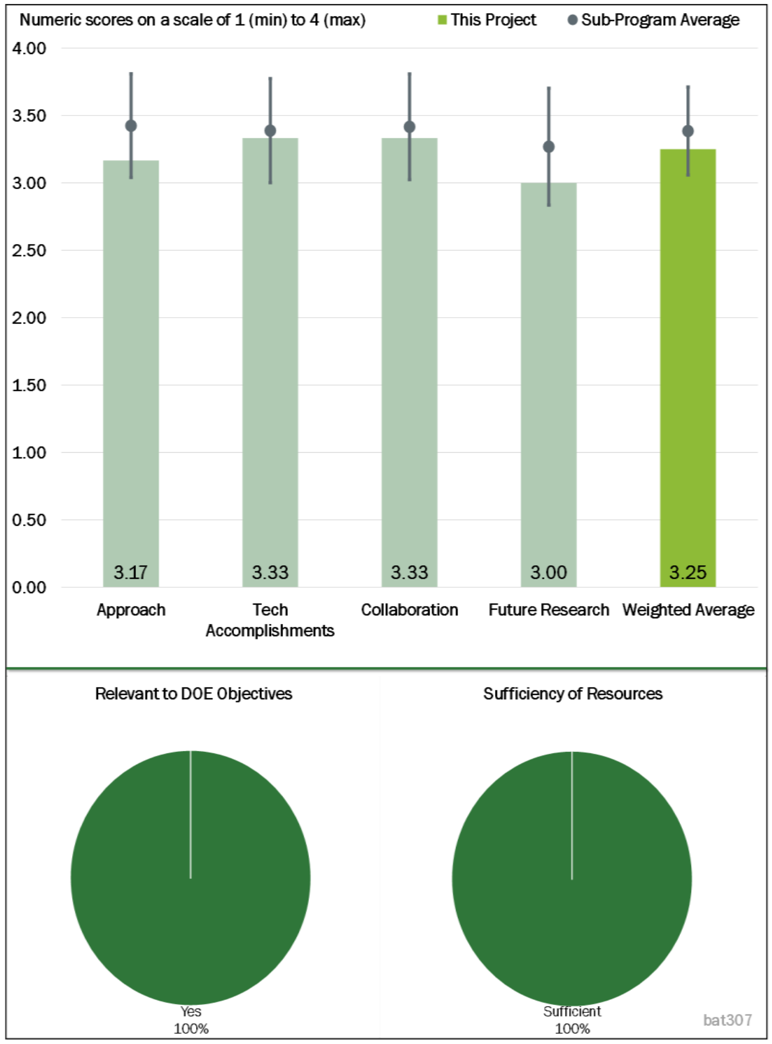

Figure 2-33 - Presentation Number: bat307 Presentation Title: Discovery of High-Energy Lithium-Ion Battery Materials Principal Investigator: Wei Tong (Lawrence Berkeley National Laboratory)

Presenter

Wei Tong, 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 and well-planned.

Reviewer 1:

The reviewer remarked that the approach of this research is to design novel Ni-based cathode materials with potentially high energy density by integrating a second TM to improve the structural stability and/or contribute electrochemically active redox. Overall, the proposed approach can break the technical barriers as mentioned in the report.

Reviewer 2:

The reviewer said that this project designs compositions that contain excess Li and utilizes Ni^{2+} to Ni^{4+} redox along with a second TM to achieve high capacity and good structural integrity. The project is investigating the impact of anionic oxygen activity on voltage fade in Li-rich metal oxides by combining DEMS, advanced synchrotron spectroscopy, and electrochemical characterization; finally, materials are designed to elucidate the potential impact of TMs on oxygen activity during electrochemistry.

Reviewer 3:

The reviewer pointed out that the research question central to this project is an important one: namely, that oxygen redox may play a critical role in voltage fade in Li-rich layered oxides. However, the results for this year focus almost exclusively on understanding the case where no oxygen redox is present. The results thus confirm the role of only transition metal (Ni and ruthenium) redox in $Li_{1.2}Ni_{0.2}Ru_{0.6}O_2$ (LNRO). The choice to work on LNRO is somewhat questionable to the reviewer because of the inherent cost barrier in using materials with ruthenium; however, in discussions during the poster session, the PI explained that this is merely a control material for comparison with high-Li nickel manganese oxide (LNMO). Some data for LNMO are presented, but comparisons are insufficient to demonstrate the desirability of oxygen redox (or not). It was somewhat interesting to the reviewer that with different Ni/ruthenium ratios, oxygen redox is still irrelevant in LNRO, a topic that could be explored further. The electrochemical characterization and XAS measurements (plus scanning transmission electron spectroscopy [STEM]) lead to somewhat speculative conclusions about the reason for voltage fade, which needs to be clarified. To the reviewer, this project should refocus on showing conclusively that voltage fade is related to the formation of a second crystal phase in LNRO and that this mechanism is either relevant or irrelevant in LNMO.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
According to the reviewer, the technical accomplishments and progress are excellent. The research proceeds in a logical manner, and many characterization techniques have been used to get to a full understanding of the structural information of the cathode materials. All of the achievements are critical to realize the overall goals of the project.

Reviewer 2:
The reviewer opined that this project found competition between TM redox and oxygen redox. Voltage fade phenomena were observed in LNRO, but at a much lower degree. The layered monoclinic structure likely contributes to voltage fade during cycling.

Reviewer 3:
The reviewer commented that a Li-rich layered oxide has been studied that does meet the go/no-go criteria of 200 mAh/g. To the reviewer, this target is not ambitious enough because commercially available NMC-622 already exceeds this at higher charge/discharge rates. Little effort seems to have been made to quantify performance metrics for LNRO like voltage fade over reasonably large numbers of cycles, which is an unfortunate oversight. One could easily argue that LNRO is not commercially relevant and that it does not help the project team study the critical question of oxygen redox in Li-rich layered oxides, but as a control, studying this material does produce some insights into cathode degradation mechanisms.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted that this project had collaboration among many national laboratories and universities as shown in the presentation

Reviewer 2:
The reviewer noted that there is work with the SSRL, the Advanced Light Source (ALS), the Advanced Photon Source, and the University of California at Berkeley (UCB).

Reviewer 3:
The reviewer stated that collaboration across the project team seems effective, but additional detail is needed on how complementary each contributor is to the larger effort.

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

Reviewer 1:
The reviewer stated that the work is planned in a logical manner.

Reviewer 2:

Overall, the proposed future work is excellent, according to the reviewer, who suggested that the PI should also pay more attention to the gassing issue. Approaches to depress the gas releasing during the battery cycling need to be addressed.

Reviewer 3:

The reviewer commented that the proposed future work is reasonable; however, after nearly 3 years, the reviewer expected that much of what is being proposed would already have been investigated. The remaining questions should have been as obvious at the beginning of this project as they are now.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer stated that the project goals including developing a cathode that can cycle greater than 200 mAh/g while exhibiting minimal capacity and voltage fade in order to gain an in-depth understanding of the correlation between composition and electrochemistry in Li-rich layered oxides.

Reviewer 2:

The reviewer commented that DOE overall target is to develop Li-ion batteries with low-cost, high energy density, and high electrochemical properties. The target of this project is consistent with DOE's goals. However, as Ni-rich NMCs reach 250 mAh/g, the PI of this project should target even higher capacity cathode materials.

Reviewer 3:

The reviewer remarked that this project does attempt to address DOE objectives concerning the development of higher energy cathode materials; however, the output could have been better given the resources and time spent.

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 the resources from many national laboratories and universities are sufficient to support the research work of this project.

Reviewer 2:

The reviewer commented that for the amount of relevant work produced in the project, the resources have been sufficient or underutilized compared to projects with similar budgets.

Reviewer 3:

The reviewer noted that this project achieved two out of four milestones.

Presentation Number: bat310
Presentation Title: Advancing Solid-State Interfaces in Lithium-Ion Batteries
Principal Investigator: Nenad Markovic (Argonne National Laboratory)

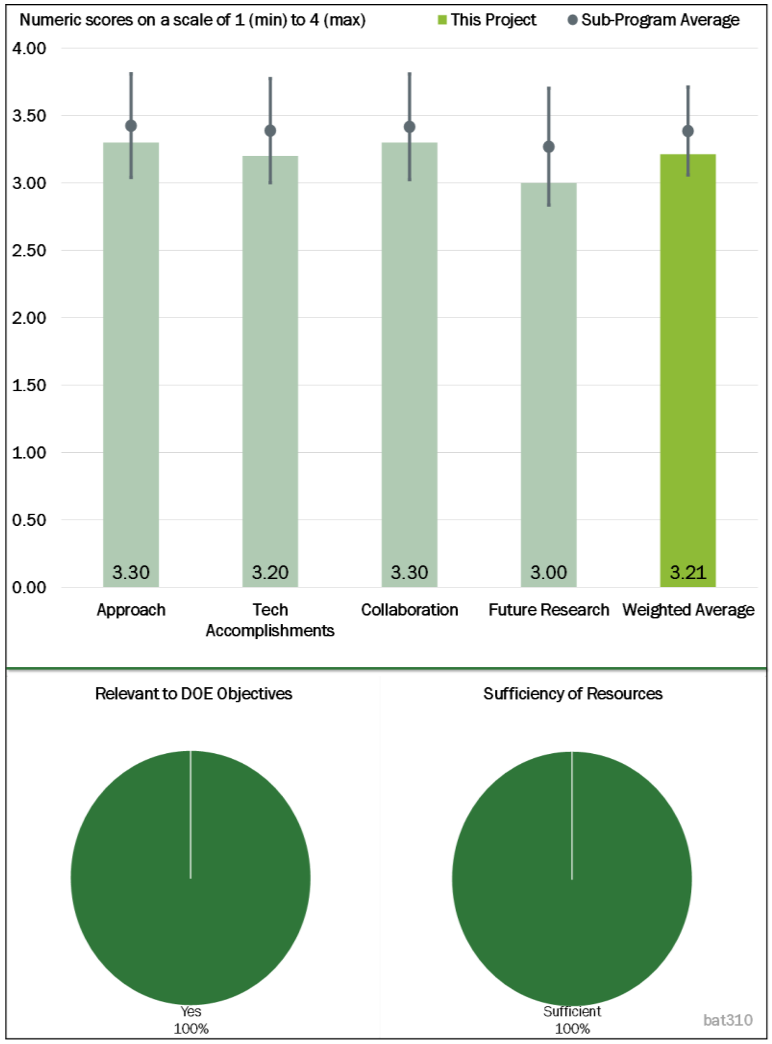

Figure 2-34 - Presentation Number: bat310 Presentation Title: Advancing Solid-State Interfaces in Lithium-Ion Batteries Principal Investigator: Nenad Markovic (Argonne National Laboratory)

Presenter

Nenad Markovic, 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 and well-planned.

Reviewer 1:

According to the reviewer, the team has done an excellent job in studying the solid-solid interfaces in Li-ion batteries. The team employed science-based, multiscale experimental, and computational approaches to develop a mechanically/chemically stable, Li-ion, conductive, nonflammable solid electrolyte. The team has successfully identified several elements that are critical for such an electrolyte. The project started in 2016, and the reviewer opined that it has made remarkable progress in addressing the technical barriers.

Reviewer 2:

The reviewer found the approach of integrating glove box, sputtering, and X-ray photoelectron spectroscopy (XPS) to be excellent. The XAS, XRD, and hard X-ray photoelectron spectroscopy (HAXPES) are all great techniques for searching for answers to the key questions of interfacial processes in rechargeable batteries. Therefore, the approach is excellent.

Reviewer 3:

The project addresses a critical need of understanding the stability of different SSEs versus Li, whether the Li is cleaned or not, and the delay in growth of impedance layers due to already formed impedance-inducing contamination layers.

Reviewer 4:

The reviewer commented that studying electrochemical interfaces for solid electrolytes will help advance solid-state battery technology, although the project scope did specify this. Using modeling tools to study a range of materials is great and helpful; however, the reviewer stated that it would be more realistic if a battery system were specifically chosen and used--for example, NMC/LLZO/lithium (all solid-state cells)—to study the materials behavior during battery cycling at room and elevated temperatures.

Reviewer 5:

The approach seemed good to the reviewer, who stated that XPS is a great method to look at the energetics. The reviewer thought that the PI should focus a little more on understanding the XPS data.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer remarked that the team has demonstrated several technical accomplishments and progress in the overall project. The project is in good shape in terms of milestones. The team has not reported much in terms of mechanics of solid electrolytes, which are important for developing mechanically robust solid electrolytes.

Reviewer 2:

The reviewer commented that the team has shown progress on the oxide structures and especially the stability versus a contaminated and non-contaminated Li source. There is still a significant amount of work to do to show stability against multiple SSE-based electrolytes and common contaminants (including moisture-based decomposition products).

Reviewer 3:

The reviewer found that very useful electrochemical data on lithium lanthanum zirconium molybdenum oxide (LLZMO) materials were generated in the program so far. Any potential impact of these material changes on cell performance should be studied in the future.

Reviewer 4:

The information generated looked good to the reviewer, who really liked the XPS data as a function of temperature. The reviewer said that the team should be able to calculate the binding energy of the surface species and suggested calculating some binding energies from these data. The data can be used with first-principle modeling (which the reviewer suggested for future work) to get a better understanding of the energetics. It seemed to the reviewer that doping is not really doing much to this structure (Slide 16), and the reviewer expected a little more change. The reviewer asked what the concentrations are.

Reviewer 5:

The reviewer stated that the overall progress of the project appears to be on track against what has been proposed. The proposed technique and approach are excellent. However, it appeared to the reviewer that the research outcome is very limited, with only one paper accepted and one under preparation. This appeared off to the reviewer when benchmarked with other projects.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the group at ANL has outstanding facilities and an in-depth knowledge of model surfaces.

Reviewer 2:

According to the reviewer, the ANL team has done a good job collaborating with DOE national laboratories and universities.

Reviewer 3:

The reviewer found all the collaboration teams to be leading experts on the proposed direction.

Reviewer 4:

The reviewer noted that the team has demonstrated several good collaborations in experimental characterization and modeling. More collaborations are needed to study the mechanics of the developed electrolytes, which must be mechanically robust as well.

Reviewer 5:

Collaboration seemed fine to the reviewer, who suggested that the team get in contact with someone doing first-principle modeling (density functional theory [DFT]) to compare some of these binding energy predictions against. This would be really interesting.

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

Reviewer 1:

The reviewer commented that the team proposes to focus on a Li solid-electrolyte system and a cathode solid-electrolyte system. These are outstanding challenges for solid-state battery system based on a Li-metal anode, SSE, and cathode.

Reviewer 2:

The reviewer indicated that the future project plan would complete the survey of all the different SSE materials and their stability against Li and Li contaminants; this is a desired result.

Reviewer 3:

The reviewer remarked that the proposed future work is well planned and suggested that the team study the microstructure and mechanical property changes during cycling. It is important to establish the relation between microstructure (grain size and defects) and chemical and mechanical properties of the developed electrolytes.

Reviewer 4:

The reviewer expressed concern with the overall method and somewhat with the technical gap between using “lithium/SSE/lithium” as a platform in modeling and using battery cells. According to the reviewer, there are some reports of Li dendrites growing through LLZO grain boundaries; meanwhile, some companies demonstrated good cycling solid-state cells without observing negative impacts of Li dendrite growth. This is a good indication that battery cell configurations, such as cathode/SSE/Li, could be a more realistic modeling platform than Li/SSE/Li.

Reviewer 5:

The reviewer recommended collaborating with someone doing DFT calculations as this might help to explain the chemistry a little better.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer affirmed that to enable Li anodes especially at higher rates, it is necessary to understand which SSE is stable against Li and what is required for surface cleaning for the lithium.

Reviewer 2:

The reviewer opined that studying SSEs on both structures and interface issues will help advancing solid-state battery technology so this project supports the overall DOE objectives.

Reviewer 3:
The reviewer remarked that high-performance solid electrolytes are greatly needed for the next generation of batteries. There are several challenges, such as chemical stability, mechanical robustness, and compatibility between the solid electrolyte and the electrode, which are less or completely unknown.

Reviewer 4:
The reviewer pronounced the project as relevant to DOE.

Reviewer 5:
The reviewer stated that solid-state batteries have been viewed as the future of the rechargeable battery for safe operation, while the interfacial process is the key. In this sense, the project rightly purged on this topic.

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 ANL has several unique instruments that are critical to the success of this project. The team has employed the combined glove box, sputtering, and XPS chamber system. Using XAS, XRD, and HAXPES is also helpful.

Reviewer 2:
The reviewer indicated that the resources appear to be commensurate with what can be done.

Reviewer 3:
The reviewer commented that the resources for the project are sufficient to achieve the stated milestones.

Reviewer 4:
The reviewer observed that the current resources are sufficient to achieve the project targets.

Reviewer 5:
The reviewer stressed doing some DFT calculations and using an HPC system to find someone who can help with first-principle calculations.

Presentation Number: bat312
Presentation Title: Advanced Lithium-Ion Battery Technology: High-Voltage Electrolyte
Principal Investigator: Joe Sunstrom (Daikin)

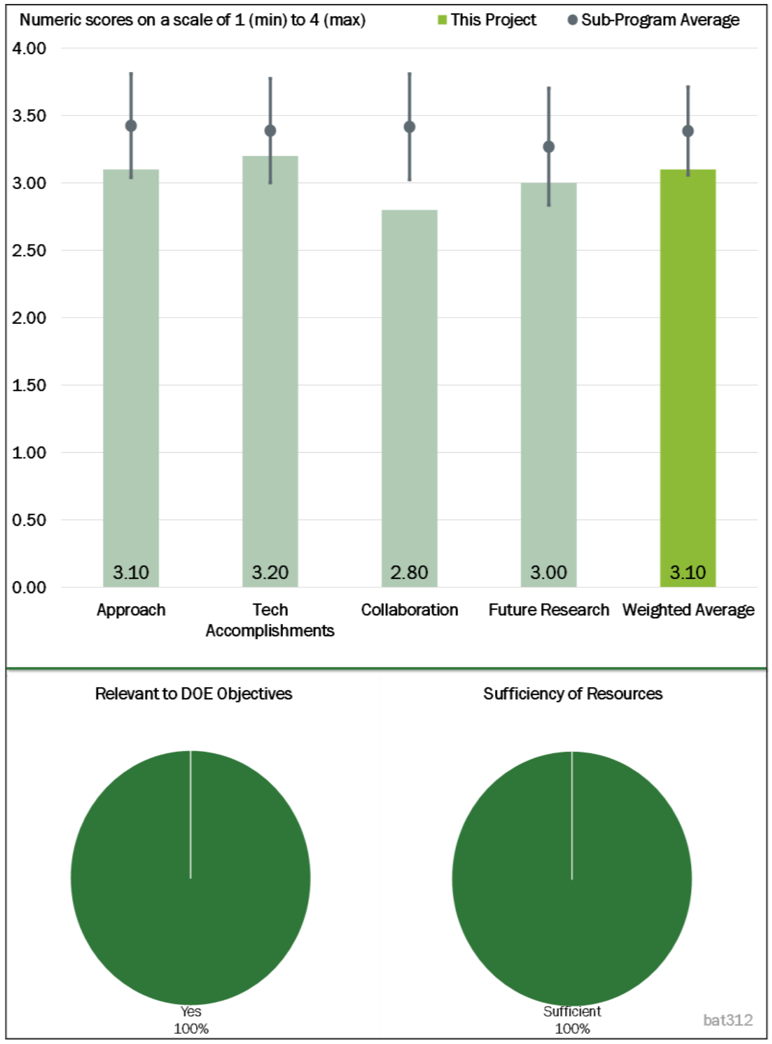

Figure 2-35 - Presentation Number: bat312 Presentation Title: Advanced Lithium-Ion Battery Technology: High-Voltage Electrolyte Principal Investigator: Joe Sunstrom (Daikin)

Presenter
Joe Sunstrom, Daikin

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 and well-planned.

Reviewer 1:
The reviewer remarked that the Daikin team has done an excellent job in developing high-voltage electrolytes for Li-ion batteries. The team has discovered several new failure mechanisms. The correlation between SEI and gas generation has been established. The project started in 2016 and has made remarkable progress in addressing the technical barriers.

Reviewer 2:
The reviewer pointed out that using fluoroethylene carbonate (FEC) additives to stabilize electrolytes at higher voltages is cost effective; however, this might not be able to fundamentally solve the problem. The maximum 4.6 V voltage range proposed in the project is somewhat low because there is 5V LNMO-C chemistry available currently. Studying gassing is useful and necessary; however, the project does not seem to establish methods to differentiate any possible gassing contributions from other cell components (binders, additives, separator coatings, as well as other cell components exposed to the electrolyte) other than the electrolytes. With its expertise in fluorine chemistry, Daikin America is a good company to develop all fluorinated electrolytes with a focus on lowering the cost.

Reviewer 3:
The approach seemed good to the reviewer, who proposed measuring the dielectric strength of the material.

Reviewer 4:
The barriers to high-voltage electrolytes are being addressed through development of an understanding of the failure mechanism. The plan for mechanistic understanding is detailed and very good. There does not seem to be a very well-designed plan for finding electrolyte additives and what there is comes at the end of the 3-year period.

Reviewer 5:

The reviewer stated that the team is focusing on exploring the stability of electrolytes for long cycle life. The main research topic appears to be focused on compatibilities between the electrolyte and the cathode for high-voltage operation up to 4.6V. Also, it was hard for the reviewer to know if the fading at high voltage is due to the failure of the electrolyte or due to the cathode itself. For the anode side, depending on the anode, the interfacial reaction will also play a big role in terms of stability.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that the team has demonstrated several technical accomplishments and progress. The project is in good shape in terms of milestones. The reviewer suggested that modeling of the electrolyte/electrode be carried out.

Reviewer 2:

The reviewer noted that it looks like the team has achieved the 4.6V target already.

Reviewer 3:

According to the reviewer, excellent progress has been made on the failure mechanisms of high-voltage electrolytes through the systematic studies. Not much progress on the development of new additives is evident.

Reviewer 4:

The reviewer indicated that it is known that gassing will take place at higher voltages for LCO/NMC/nickel cobalt aluminum oxide (NCA) cells. The project generated some useful data regarding gas composition, etc. Although gassing in cells is a messy, complicated problem, the project should at least make an effort to speculate about what the various sources are and the mechanisms to explain the gas composition.

Reviewer 5:

The reviewer said that the team has made some good progress in analyzing the composition of the gas, while the overall work appears to have been carried out in a trial-and-error manner. The major weak point is the lack of a fundamental hypothesis and proof of concept. A systematic approach may be complementary to the trial-and-error method.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that the collaboration seems good, and Daikin seems interested in doing the research.

Reviewer 2:

The reviewer encouraged the team to reach out more to collaborate with other groups to work on the surface of both the cathode and anode. A collaboration with a microscopy group to study the surface of both anode and cathode as a variation of electrolyte chemistry could be very beneficial to the project.

Reviewer 3:

The reviewer found not much in the way of collaboration. However, that is understandable as most of the characterization is being done in-house.

Reviewer 4:

The team did not show any collaboration with national laboratories and universities, according to the reviewer, who suggested that the team reach out to collaborate with modeling groups at national laboratories and universities.

Reviewer 5:
The reviewer stressed that, even not as formal project subcontractors, national laboratories and universities should be involved more in the project to help with the electrolyte-degradation study.

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

Reviewer 1:
The reviewer said that the proposed future work is within the project scope and there are some efforts proposed on collaboration with outside resources.

Reviewer 2:
The reviewer found the proposed future work to be well planned, and suggested that the team study the atomistic-/molecular-level interactions between the electrolyte and the electrode during/after cycling at high voltages.

Reviewer 3:
The reviewer urged the team to keep going, run more experimental tests, and consider any health or environmental hazards that might impede this technology from making it into the consumer market.

Reviewer 4:
The reviewer remarked that the proposed research for this project is largely on failure mechanisms and the characterization approaches. It seems to lack much in the way of plans for the development of electrolyte additives.

Reviewer 5:
The reviewer pronounced the proposed research as good, but as the research converges towards the end of the project, the team should be more hypothesis driven based on what has been learned rather than still trial-and-error. Computable electrolyte computable for both cathode and anode needs to be considered from this reviewer’s perspective. By focusing only on cathode electrolytes, the reviewer was very dubious about whether the optimized electrolyte will work or not for the case of the anode side.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer stated that the overall objective of optimizing the electrolyte towards high-voltage operation of the battery is very relevant for VTO.

Reviewer 2:
The reviewer commented that high-performance electrolytes facilitate stable, high-voltage cycling of Li-ion batteries, presenting a pathway to higher energy batteries that is beneficial towards DOE cost targets ($/kWh).

Reviewer 3:
The reviewer said that stabilizing electrolytes at higher voltages helps extend battery life and increases cells’ energy density. This project supports the overall DOE objectives.

Reviewer 4:
The reviewer commented that the research is relevant to the DOE objective of finding electrolytes to enable high-voltage cathodes.

Reviewer 5:
The reviewer said that the project was relevant to DOE.

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 resources for this project are sufficient to achieve the stated milestones.

Reviewer 2:
The reviewer indicated that resources at Daikin are sufficient.

Reviewer 3:
The reviewer said that the resources are good as compared with other, similarly scaled work.

Reviewer 4:
The team has fully used the resources at Daikin, according to the reviewer, who suggested that the team reach out to national laboratories and universities to do modeling.

Reviewer 5:
The reviewer stated that there are good resources and encouraged measuring the dielectric strength of the electrolyte.

Presentation Number: bat319
Presentation Title: Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte
Principal Investigator: Shirley Meng (University of California-San Diego)

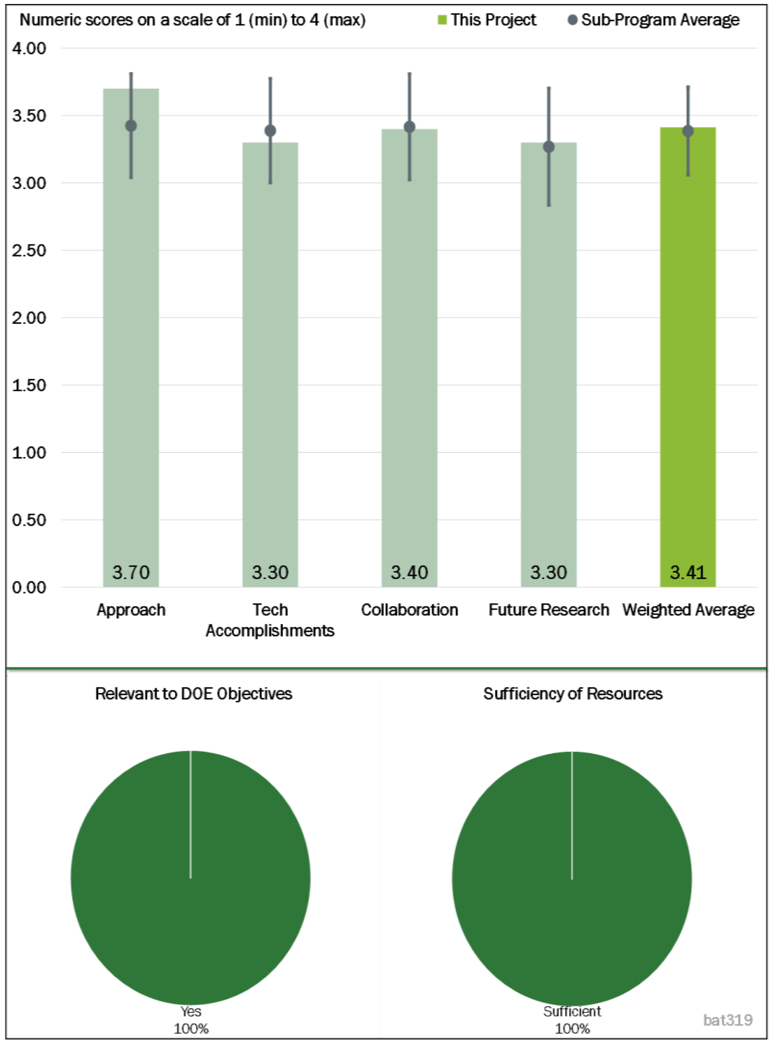

Figure 2-36 - Presentation Number: bat319 Presentation Title: Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte Principal Investigator: Shirley Meng (University of California-San Diego)

Presenter

Minghao Zhang, University of California-San Diego

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 and well-planned.

Reviewer 1:

The reviewer praised the team's excellent work in studying electrode/electrolyte interphases in Li batteries. The team uncovered the anion redox and oxygen evolutions in Li-excess NMC materials and tracked the Li and oxygen dynamics under electrochemical testing. The study on the chemical composition and structure of electrochemically deposited Li metal is of great interest. The project started in 2016 and has made remarkable progress in addressing the technical barriers.

Reviewer 2:

The reviewer said that there is a good combination of state-of-the-art characterization techniques to probe anion redox and oxygen evolutions in Li-excess NMC materials. In addition, in-operando neutron diffraction will be used to study dynamics and strategies for synthesis of modified cathode materials are proposed.

Reviewer 3:

The reviewer found that very useful microscopy and spectroscopy techniques for probing battery electrodes have been demonstrated in this program. The lithium lanthanum titanate (LLTO) coating on the Li-rich, layered-oxide cathode materials is a good idea, and the same concept could be used on other cathode materials as an effective way to improve cells' cycle life.

Reviewer 4:

The reviewer commented that the approaches include a combination of microscopy, neutron scattering, and X-ray diffraction. All these cutting-edge techniques reveal certain aspects of information about battery materials. Therefore, an integrated use of these different techniques will help to capture complementary information for understand battery failure.

Reviewer 5:
The approach seemed good to the reviewer, who pronounced the experimental methods to be appropriate.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer remarked that excellent progress has been made on probing various aspects of electrode-electrolyte interphases, including Li-rich oxides and coatings. The characterization techniques are yielding useful information.

Reviewer 2:
The reviewer commented that this proposed work is an excellent addition to the toolbox of current battery research and development. The project generated very useful data that will shed light on battery-materials optimization.

Reviewer 3:
The reviewer stated that the team has demonstrated several technical accomplishments and progress in the overall project. The project is in good shape in terms of milestones. The reviewer suggested carrying out modeling of the electrolyte/electrode interphases.

Reviewer 4:
Accomplishments seemed fine to the reviewer, who was not sure about the point of being able to reheat the cathode material to regenerate it. The reviewer said that the PI should think about how to stabilize the phase, and maybe what substrates may stabilize the phase.

Reviewer 5:
The reviewer noted that the diagnostic results provide certain insights on the degradation mechanism of a Li-rich cathode. However, the reviewer was very doubtful about the heat-treatment scheme for resolving the fading problem of this category of cathode or, in other words, how the heat-treatment strategy can be used for a battery system to resolve the fading problem.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
According to the reviewer, excellent collaboration and coordination across the project teams has been achieved in this program.

Reviewer 2:
The reviewer pointed out that the team has a good collaboration with teams that have different skill sets.

Reviewer 3:
The reviewer noted that numerous collaborations enhance the project.

Reviewer 4:
The reviewer acknowledged that the team has been collaborating with national laboratories and universities and suggested that the team reach out to collaborate with modeling groups at national laboratories and universities.

Reviewer 5:
Collaboration seemed good to the reviewer. There was mention of potentially doing some DFT calculations. The reviewer suggested that the PI collaborate with an expert who has experience doing DFT calculations. This would be a better use of resources instead of the PI having their students learn how to use DFT software.

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:

To the reviewer, the plans for the Li-rich layered oxide (LRLO) materials as well as the Li anode seem well defined and make use of state-of-the-art characterization methods. The theory does not seem well integrated yet, and it is not clear how the DFT methods can be used to study heat treatment in these materials.

Reviewer 2:

The proposed future work is well planned, according to the reviewer who suggested that the team study the atomistic-/molecular-level interactions between the electrolyte and the electrode during/after cycling at high voltages.

Reviewer 3:

The reviewer remarked that the proposed future work is within the project scope and well planned. The reviewer is concerned, however, by the effort/focus on "recovering" the structures and voltage of LRLO materials. Recovering the LRLO structures, using either thermal or pressurizing methods, is some post-processing for battery materials, not something realistic for a fabricated cell in service or being beneficial to overall cell performance. Focusing on improving LRLO or other cathodes performance in cells by nanometer coatings, etc., will make this program very relevant and more productive. The reviewer, however, understands that this is probably not part of the original work plan.

Reviewer 4:

The reviewer proposed focusing on stabilizing the phase and asked what substrates can be used to help stabilize the phase. The reviewer would also use DFT to help understand the stability in order to calculate the formation energy of the phase deposited on different substrates. The reviewer would not mess with the nudged elastic band method. Again, the reviewer suggested that the PI collaborate with someone who has experience conducting DFT simulations.

Reviewer 5:

The proposed future research appeared to the reviewer to be on track with the overall objectives of the proposed research. However, the reviewer was very conservative regarding the method of heat treatment and high-pressure treatment for resolving the fading problem. The reviewer asked how these two methods can be implanted in an assembled battery.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer found the proposed research to be very relevant to DOE objectives. Finding the fading mechanism and a way of mitigating the fading of the cathode is critical to advancing battery technology for electrified cars.

Reviewer 2:

The reviewer stated that understanding the electrode/electrolyte interphases in Li batteries is critical to achieve the goals of an energy density of 500 Wh/kg and 1,000 charge/discharge cycles.

Reviewer 3:

The reviewer commented that this program strongly supports the overall DOE objectives.

Reviewer 4:

The reviewer said that the project supports the development of new battery materials.

Reviewer 5:
The reviewer affirmed that the project is relevant.

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

Reviewer 1:
The team has fully used the resources at the University of California at San Diego, DOE national laboratories, and Cornell University, according to the reviewer, who suggested that the team reach out to national laboratories and universities to do modeling.

Reviewer 2:
The reviewer noted that the current resources of this program are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 3:
The reviewer reported that an appropriate amount of resources is assigned to this project.

Reviewer 4:
The reviewer remarked that the resources are sufficient.

Reviewer 5:
The reviewer pronounced resources to be good, and asked that the team please use the HPC system to run DFT calculations.

Presentation Number: bat321
Presentation Title: Solid-State Inorganic Nanofiber Network-Polymer Composite Electrolytes for Lithium Batteries
Principal Investigator: Nianqiang Wu (West Virginia University)

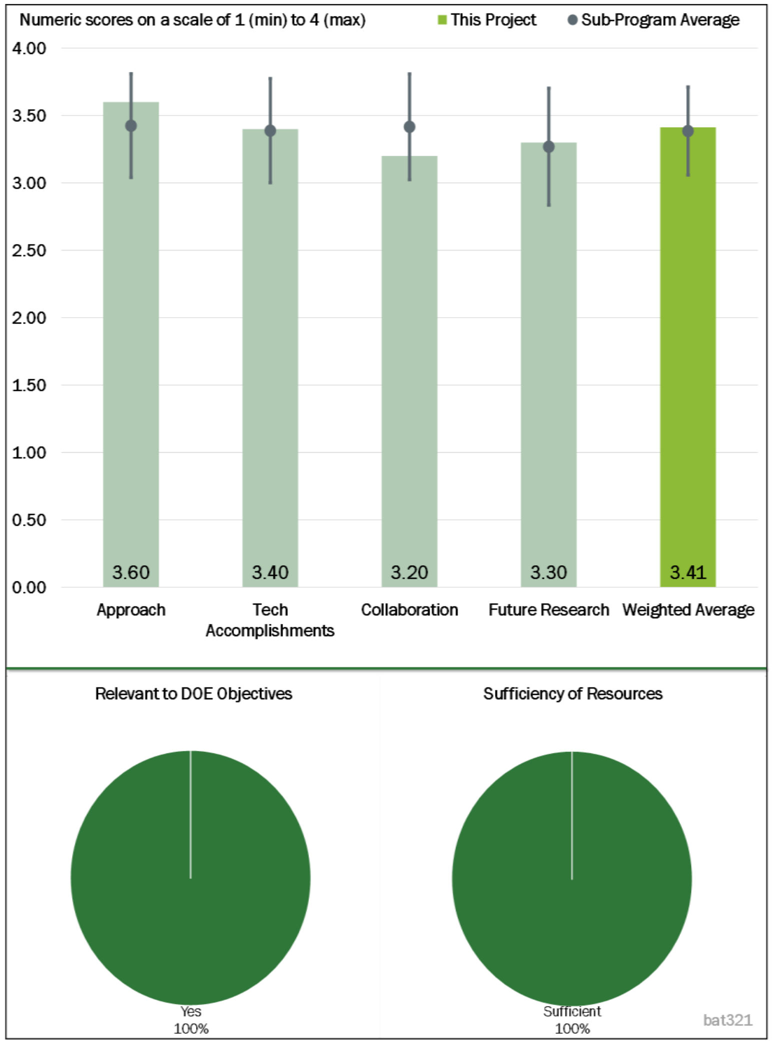

Figure 2-37 - Presentation Number: bat321 Presentation Title: Solid-State Inorganic Nanofiber Network-Polymer Composite Electrolytes for Lithium Batteries Principal Investigator: Nianqiang Wu (West Virginia University)

Presenter

Nianqiang Wu, West Virginia University

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 and well-planned.

Reviewer 1:

The reviewer stated that the technical approach is very good as it addresses one of the key technical barriers addressing Li-metal rechargeable batteries. The ionic conductivity of these solid-polymer electrolytes is relatively low, and this therefore severely hinders their use in Li-metal batteries. The PI is attempting to decrease the crystallinity of polymers by the addition of inorganic nanofibers, which the reviewer opined should improve ionic mobility and lay out a feasible path.

Reviewer 2:

The reviewer remarked that the approach, based on a composite electrolyte of a polymer matrix and inorganic fibers, is part of a strategy to address both ionic conductivity and interfaces needed for good SSEs. The approach is well designed and worthwhile to try as it could overcome problems with ionic conductivity of polymers at room temperature as well as interface problems.

Reviewer 3:

The reviewer called the design of the composite electrolyte system very nice and technically sound. The ultraviolet (UV) curing process makes the whole separator system very versatile and practical.

Reviewer 4:

The reviewer commented that the approach in this project involves fabrication of a hybrid solid electrolyte, based on polymer matrix and inorganic fibers with high ionic conductivity and mechanical robustness. An interesting aspect of the approach is the in situ polymerization of the electrolyte on the surface of a cathode, which can enable better cathode/electrolyte interface. In this approach, the electrolyte is in its liquid form, and it can penetrate through pores in a composite cathode leading to the increased cathode/electrolyte contact area and overall improved electrochemical performance of the battery. This is not needed for the anode/electrolyte interface as the anode is a metallic Li with no pores.

Reviewer 5:

The reviewer said that the main objective of this work is to develop a polymer matrix and inorganic, composite SSE for a full solid-state battery. The reviewer liked the idea of this type of composite. The project team currently intends to increase the ionic conductivity of both inorganic and polymer materials to enhance the composite ionic conductivity. This is logically correct. In the reviewer's opinion, the interface between the matrix and the dispersed inorganic particle will be also critical, which has been demonstrated for the case of a high-temperature oxygen conductor.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that good progress has been achieved thus far. The group has synthesized three precursors and monomers for block co-polymers, and has also prepared a block co-polymer, and synthesized three different types of inorganic nanofibers. The team appears to be on schedule.

Reviewer 2:

The reviewer said that the work was systematically conducted, with a combination of experimental and theoretical calculations. The reviewer liked the step-by-step approaches, and the composite electrolyte made so far shows stable cycling based on Li metal and LFP.

Reviewer 3:

The reviewer remarked that very good cell results were demonstrated using a composite solid-state separator system, and the solid-state electrolyte showed much improved ionic conductivity and mechanical properties over other SSE. The demonstrated UV-curable process for fabricating the cathode is particularly interesting. The interfacial issues generally associated with solid-state batteries were nicely mitigated in this project.

Reviewer 4:

The reviewer commented that progress has been made in the synthesis of polymers and inorganic fibers with good conductivity and stability properties. However, the composites still do not have the necessary ionic conductivity; the idea that the nanofibers would decrease crystallization does not appear to have solved the conductivity problem of the polymers.

Reviewer 5:

The reviewer said that, first, a salt-added, cross-linked polymer, Li electrolyte with the ionic conductivity of 2.40×10^{-4} Siemen per centimeter (S/cm) was synthesized, thus reaching a goal for the polymer matrix conductivity. Second, measurements of ionic conductivity in the Al- and nitrogen-doped LLTO inorganic nanofibers revealed that 0.5% aluminum-doped LLTO exhibited the highest ionic conductivity (1.08×10^{-3}S/cm) of all synthesized samples, thus reaching a goal for the inorganic fibers conductivity. Third, a composite electrolyte made of a cross-linked polymer matrix and inorganic fibers was fabricated. It was shown that the addition of inorganic fibers improved mechanical properties and the Li transference number of the polymer matrix.

The reviewer posed several questions. Despite the fact that the ratio between the polymer matrix and inorganic fibers was varied, it remained unclear to the reviewer how both ionic conductivity and mechanical properties of the composite electrolyte change as the ratio between polymer and fibers changes. The reviewer wanted to know if there is an optimum ratio that provides the highest ionic conductivity and best mechanical robustness, including suppression of lithium dendrite growth. Next, the reviewer stated that the goal to understand the mechanism of ion transport that involves three alternative routes—Li transport through polymer matrix, Li transport through inorganic fibers, and Li transport at the interface between the polymer component and fibers—is important to design and fabricate solid electrolytes with best electrochemical performance. The team is encouraged to test composites made of non-conductive polymer and conductive inorganic fibers with different ratios between the polymer and fiber components to evaluate electrochemical performance of fibers only. The reviewer pointed out that there is only one paper reported to be published during the reporting period. To strengthen the team's appearance in the solid-electrolyte community, the reviewer encouraged the team to publish more. Given the number of the reported manuscripts under preparation, this seems not to be an issue in the future; however, at the moment the number of published papers is not high.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found that the project demonstrated good collaboration and coordination across project teams.

Reviewer 2:

The reviewer remarked that the project has several collaborations, including for theory and synthesis,

Reviewer 3:

The reviewer noted that collaboration exists with North Carolina State University.

Reviewer 4:

The reviewer stated that the project lead is West Virginia University, and all types of experiments can be and are being conducted at this institution. The key partner, North Carolina State University, provides complimentary investigation of polymer matrix design, synthesis, and characterization as well as full cell testing. It would be helpful if the PI added the name of the partner to evaluate collaborative publications.

Reviewer 5:

The reviewer stated that the project team is collaborating with a theoretical group and other two groups. In the reviewer's opinion, the team can collaborate more widely with other battery groups to extend to other possible materials system both in the polymer and inorganic particles.

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 remarked that future efforts are logical and justified by the results thus far. The project team will optimize and develop new polymers and modify the ceramic nanofiber surface to create a buffer layer at the ceramic-polymer interface.

Reviewer 2:

The reviewer said that the proposed future research addresses the key barriers of the project. The team proposal to focus on enhancing both the bulk and interfacial conductivity is the right approach.

Reviewer 3:

The reviewer observed that the future plans of the project include improvements in polymers, inorganic nanofibers, and composites. The plans for the most part are sensible, but plans for improving the conductivity of the polymer are not well defined.

Reviewer 4:

For the project PI's consideration, the reviewer suggested the following in future work to further validate the proposed technology: Demonstrate other battery formats, such as pouch cells; demonstrate multi-layer pouch cell configuration and performance; demonstrate that the solid-electrolyte system can be used for LCO, NMC, NCA, and other chemistries; and finally and most importantly, evaluate the cell performance and report cell performance based on cell weight, kWh/kg per cell.

Reviewer 5:

The reviewer said that the team proposes further increasing the ionic conductivity of their composite electrolyte using strategies such as doping of inorganic nanofibers, applying highly conductive coatings, and modifying the interface. Additionally, the team proposes to test symmetric and full cells. In order to develop a composite electrolyte with the performance best suited for commercial batteries, the reviewer opined that it is important that the team understands better the role of the polymer matrix/inorganic fibers interface and develops ways to control this interface. The strategies proposed by the team, combined with their proposed efforts to investigate the mechanism of Li transport, make up a good plan. The reviewer encouraged the team to test multiple cathode materials and different cathode compositions with varying porosity to take advantage of their in situ polymerization approach. Additionally, the team needs to demonstrate results on Li-dendrite growth suppression with their best performing electrolytes.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer remarked that the work is highly relevant. Solid electrolytes are considered promising materials candidates to eliminate dendritic growth in Li-metal anode batteries.

Reviewer 2:

The reviewer commented that the research is relevant to the DOE efforts in developing safer, high energy density, high power density, solid-state batteries with metallic Li anodes. This project addresses development of highly conducting and mechanically stable, solid-composite electrolytes.

Reviewer 3:

The reviewer indicated that this project strongly supports the overall DOE objectives.

Reviewer 4:

The reviewer said that SSEs are an important focus for DOE VTO.

Reviewer 5:

According to the reviewer, the future success of solid-state batteries critically depends on the discovery and fabrication of solid electrolytes. Exploring solid electrolytes based on a composite polymer with inorganic polymers is a great idea; a similar principle has been demonstrated for the case of oxygen-ionic conductors.

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 team has sufficient resources to successfully meet the milestones.

Reviewer 2:

The reviewer said that the resources on this project are sufficient to achieve the stated milestones.

Reviewer 3:

The reviewer remarked that the resources are adequate for the proposed research.

Reviewer 4:
The reviewer commented that the resources available for the team are adequate.

Reviewer 5:
The reviewer observed that the resources are adequate.

Presentation Number: bat322
Presentation Title: High Conductivity and Flexible Hybrid Solid-State Electrolyte
Principal Investigator: Eric Wachsman (University of Maryland)

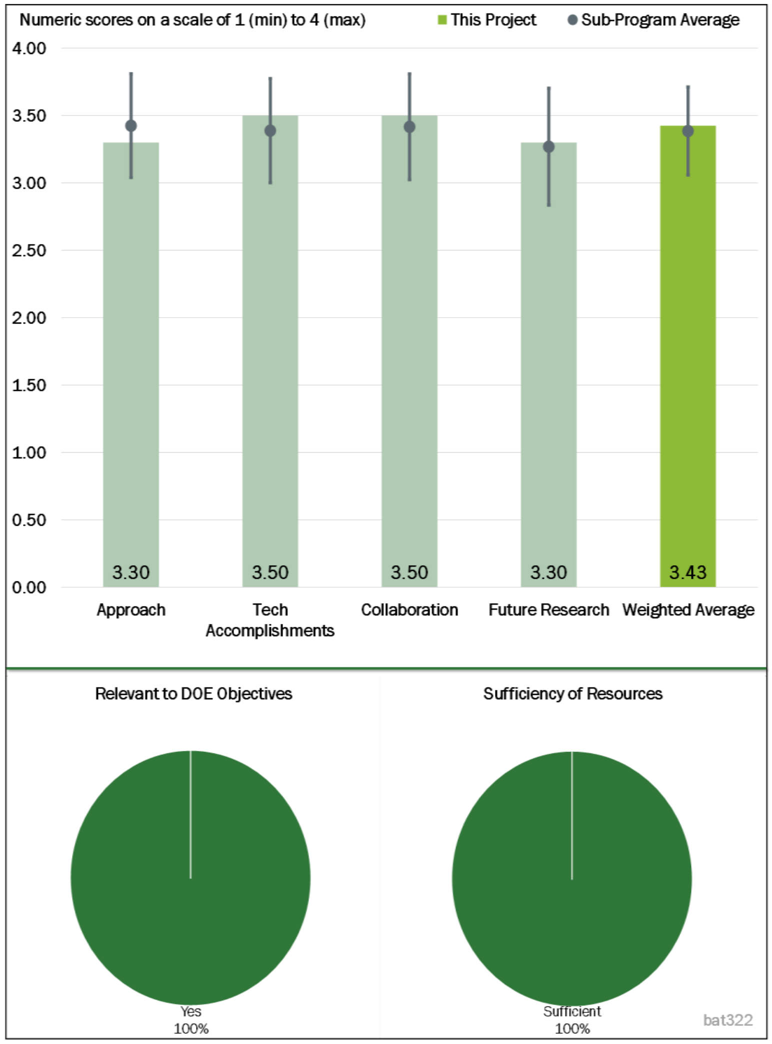

Figure 2-38 - Presentation Number: bat322 Presentation Title: High Conductivity and Flexible Hybrid Solid-State Electrolyte Principal Investigator: Eric Wachsman (University of Maryland)

Presenter

Eric Wachsman, University of Maryland

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 and well-planned.

Reviewer 1:

The reviewer noted that the approach in this project involves fabricating a hybrid solid electrolyte based on a polymer matrix and inorganic garnet fibers, with high ionic conductivity and mechanical robustness. The choice of garnet structures for inorganic fibers is highly promising, as this class of materials shows high performance as solid electrolytes. The reviewer praised the combined modeling and experimental approach to characterize Li-ion diffusion, mechanical properties, and a potential of the developed hybrid SSE to suppress lithium-dendrite growth as excellent.

Reviewer 2:

The reviewer said that the team employed a combined experimental/computational approach to developing a solid, flexible electrolyte to enable high-performance Li-ion batteries with the goal of achieving an energy density of 450 Wh/kg. The team has developed a garnet textile-reinforced, hybrid composite-polymer electrolyte. The project started in 2016 and has made remarkable progress in addressing the technical barriers.

Reviewer 3:

The reviewer remarked that this project aims to develop composite solid electrolytes based on polymer and garnet fibers. The approach is to integrate experimental with computational modeling. The reviewer stated that the computational predicated results are very interesting; the team could use this modeling result to guide the designing of better materials. Typically, it appears that the surface and grain boundary will play a big rule in contributing to ionic conduction. Therefore, the reviewer said that the work can be further extended to modify the interface and grain boundary to get better ionic conduction.

Reviewer 4:

The reviewer noted that solid-state anode development is critical to meet specific energy, energy density, cost, and life goals. So, the approach is well defined for the technical solutions.

Reviewer 5:

The reviewer observed that the project addresses the ability of taking a typically rigid SSE (garnet) and making it flexible by combining it with another polymer-based electrolyte and providing unique processing to enhance conductivity through the layer. The reviewer had reservations about this approach: by utilizing a hybrid electrolyte, the project is addressing one issue but creating many more due to all the known problems with PEO.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that the characterization and building of the electrolyte film are on target.

Reviewer 2:

Based upon the goals of the project, the reviewer reported that the PI has definitely achieved the targets, although this would not be a real-world solution due to the issues with PEO.

Reviewer 3:

The reviewer indicated that the team made great progress in fabricating the flexible hybrid electrolyte. At the same time, computation results are excellent, which provide key insights regarding the factors that may affect the ionic conduction. It should be beneficial if the team can use the modeling results to guide the design of a new composite structure for optimization of ionic conduction. Therefore, the present reviewer suggests a better integration of experiments with modeling.

Reviewer 4:

The reviewer stated that the team has demonstrated several technical accomplishments and progress in the overall project. The project is in good shape in terms of milestones. The team has not reported much in terms of mechanics of such flexible solid electrolytes. The reviewer suggested that tensile and penetration/puncture tests be carried out on the developed electrolytes.

Reviewer 5:

The reviewer summarized the progress by stating that the team demonstrated successful preparation and characterization of garnet fibers, as well as processing of the prepared fibers into a garnet textile and used garnet fibers to fabricate a hybrid composite polymer electrolyte. The team demonstrated that Li-ion conductivity of the hybrid solid electrolyte is dominated by the Li transport through the garnet fibers rather than polymer matrix. The synthesized-polymer, garnet-fiber hybrid electrolyte demonstrated good conductive and mechanical properties. The reviewer noted that hybrid SSEs with a thickness of 20 microns was fabricated using a hot press, meeting one of the goals of the proposed research. The computational study on Li-dendrite growth in the cells containing the developed hybrid SSE with garnet fibers revealed not only the effect of the presence of the fibers in the polymer matrix but also demonstrated how defect chemistry in garnet can affect formation of lithium dendrites. These results are important for both finding the best polymer matrix/inorganic fibers ratio and optimizing garnet-fiber chemistry to achieve the best hybrid solid-electrolyte performance.

The reviewer pointed out that it would be desirable to know the details of the chemistry of the polymer component of the hybrid solid electrolyte as well as the role of the polymer matrix in the overall performance of the hybrid electrolyte, such as ionic conductivity, mechanical robustness, and suppression of Li dendrites growth. The reviewer encouraged the development of the hybrid electrolyte with the fraction of the fibers oriented perpendicular to the electrode because the project showed that Li transport is dominated by Li diffusion through inorganic fibers. Development of the hybrid solid electrolyte with such architecture would maximize ionic conductivity. However, for mechanical robustness, a fraction of the fibers need to be oriented parallel to the electrodes. The reviewer thought it would be exciting to see a study on controlling the ratio of fibers oriented parallel and perpendicular to the electrodes with an evaluation of their Li-ion conductivity and mechanical strength. Such a study would be very novel and potentially impactful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the team has a good background, understanding, and phenomenal resources to make innovative solutions for solid-state batteries.

Reviewer 2:
The reviewer found the collaboration with the researchers to be good.

Reviewer 3:
The reviewer mentioned that the team consists of three PIs with complementary expertise and there is excellent coordination among team members, all located at the same university. Professor Wachsman focuses on the experimental development of the garnet fibers with optimized ion conductivity and mechanical strength, Professor Mo provides computational predictions of mechanical and conductive properties, and Professor Hu develops hybrid electrolytes and characterizes full cells with the best performing hybrid SSE. In addition, the team partners with Professor Thangadurai, co-inventor of garnet fibers, whose vision and consultation might be helpful for the performable project. Information on the team publications was not provided, making it difficult to evaluate the status of collaborative publications.

Reviewer 4:
While the team is composed of three parties within the University of Maryland and one external collaborator, the reviewer suggested that it would be beneficial to extend the collaboration to other groups. One potential collaborator will be Professor Wu from West Virginia University, who is working on a BMR project with a similar concept of making composite electrolytes of polymers and inorganic materials.

Reviewer 5:
The reviewer said that the team has demonstrated several good collaborations in experimental synthesis and characterization and modeling. More collaborations are needed to study the mechanics of the developed electrolytes (tensile and penetration tests).

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 remarked that the future plan is to do more testing on the structure and integrate it into a non-symmetrical cell. This is very relevant and will uncover many of the integration issues that were previously discussed; in addition, this will provide the research team a chance to produce another innovative solution.

Reviewer 2:
According to the reviewer, the future research will be focused on the experimental characterization of the Li-dendrite growth in the cells containing the developed hybrid SSE with garnet fibers and the development of the full Li-sulfur cells with an energy density of 450 Wh/kg.

Reviewer 3:
The reviewer saw the future research as very well focused.

Reviewer 4:

The reviewer said that the proposed research appears to have specific objectives: one is modeling and the other is experimental. The reviewer perceived that a close integration of modeling results with experiments is missing.

Reviewer 5:

The reviewer commented that the proposed future work is well planned and suggested that the team study the mechanical property changes during and after cycling.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer found the research to be relevant to the DOE efforts in developing safer, high-energy density, high-power density, solid-state batteries with metallic Li anodes, including Li-sulfur batteries that can be processed within the existing battery-manufacturing infrastructure. This project particularly addresses the development of highly conducting and mechanically stable solid-composite electrolytes.

Reviewer 2:

The reviewer said that the solid-state hybrid electrolyte will meet DOE energy targets and will reduce costs.

Reviewer 3:

The reviewer remarked that the proposed research is relevant to the DOE objective of developing better batteries for the next-generation electric car. One of the barriers is the solid electrolyte, and this research topic just serves this topic.

Reviewer 4:

The reviewer noted that high-performance, flexible solid electrolytes are greatly needed for the next-generation batteries. There are several challenges, such as chemical stability, mechanical robustness, and compatibility between the solid electrolyte and the electrode that are less or completely unknown. The project is timely and of great interest.

Reviewer 5:

The reviewer affirmed that to enable the use of garnet-based electrolytes utilizing traditional low-cost processing, an ability to make them flexible and rollable must be developed.

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 $1.4 million should be able to support the work described in the project.

Reviewer 2:

The reviewer mentioned that three PIs have fully used the resources (experimental and computational facilities) at the University of Maryland and the University of Calgary (collaborator).

Reviewer 3:

The reviewer said that the current resources are sufficient to achieve the project goals.

Reviewer 4:

The review commented that the resources available for the team are adequate.

Reviewer 5:

The reviewer stated that the resources are sufficient for the proposed research.

Presentation Number: bat323
Presentation Title: Self-Forming Thin Interphases and Electrodes Enabling 3-D Structured High Energy Density Batteries
Principal Investigator: Glenn Amatucci (Rutgers University)

Presenter
Glenn Amatucci, Rutgers University

Reviewer Sample Size
A total of five reviewers evaluated this project.

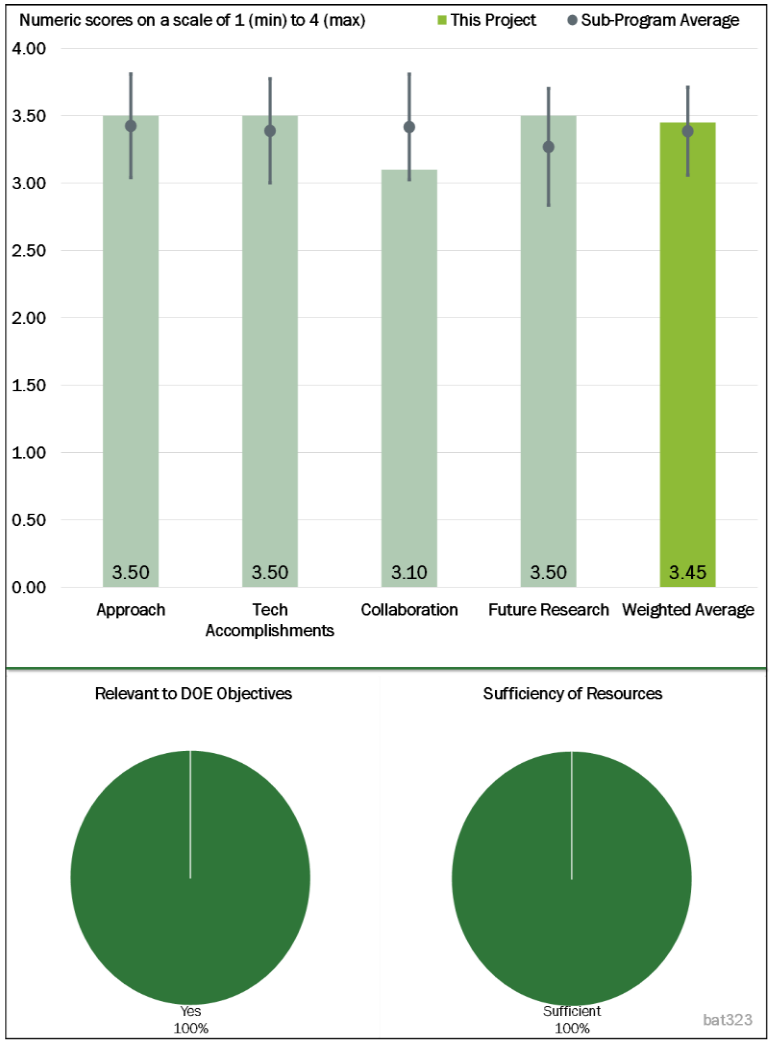

Figure 2-39 - Presentation Number: bat323 Presentation Title: Self-Forming Thin Interphases and Electrodes Enabling 3-D Structured High Energy Density Batteries Principal Investigator: Glenn Amatucci (Rutgers University)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
According to the reviewer, the development/optimization of positive/negative reactive current collector, bi-ion conductor, and battery engineering and design are the keys to developing and implementing the Li-metal-based, metal-fluoride battery. The project is well designed and feasible. It addresses composition and scalable fabrication along with composition and microstructure to facilitate rapid and uniform Li deposition during the formation cycle and subsequent cycling. It also addresses a lithium-fluoride--based composition to enable facile electrolytic decomposition at the interface that will release the F^- and Li^+ ions to react with the positive and negative current collectors respectively, thereby forming the cell in situ while maintaining a fast ionic conductor of Li^+ to facilitate subsequent cycles. In a word, most barriers are addressed based on the designed approach.

Reviewer 2:
The reviewer commented that the team developed and successfully utilizes an elegant approach to fabricate a 3-D structured, high-energy battery through a self-forming process using a bi-ion solid-state conductor comprised of a Li-fluoride-based nanocomposite glass. This bi-ion conductor releases fluorine and Li ions that react with positive and negative current collectors forming the electrodes, while the remaining fraction of the bi-ion conductor serves as a solid electrolyte. The anode in this electrochemical system is metallic Li. The cathode chemistry enables versatility through the formation of metal fluorides exhibiting high energy density, conversion-type electrochemistry due to the possibility of reacting with more than one Li ion during battery operation.

Reviewer 3:

The reviewer found this to be a good approach to developing a self-forming, solid-state battery. The chemistry is very challenging, very high risk, and high reward, which is what DOE should be funding.

Reviewer 4:

The reviewer noted that this project aims to develop and optimize the cell through the following three approaches: A nanolayered structured positive current collector, a negative current collector that enables high efficiency Li plating and stripping, and bi-ion Li-fluoride-based conductors. This project provides a well-designed approach to address the transport barriers, low utilization of a positive reactive current collector, and low efficiency of Li plating and stripping the negative current collector to achieve high energy density. It will be good if characterization tools are included.

Reviewer 5:

It was not exactly clear to the reviewer what the PI is trying to do. The chemistry is never completely mapped out nor were the specific challenges of that chemistry explained. Perhaps everything the team is doing falls under "intellectual property," but it is hard to review this work with only a vague sense of what the team is trying to accomplish.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer enthused about the wonderful progress that has been made in this project, including increasing the energy density from 25 Wh/l to greater than 570 Wh/l, the positive reactive current collector utilization from 1% to greater than 60%, and the rates in the C/2-C/20 range by two orders of magnitude The capacities and capacity retention also show great improvements.

In this project, the reviewer noted that the electrolytic method is used to form a solid-state rechargeable battery and the bi-ion Li-fluoride-based conductor. The presented in situ method is really facile, and it can bring substantial progress in the reactive current collector, which increases the efficiency for the negative current collector according to the results achieved in FY 2017. The reviewer mentioned that the project achieved a dramatically increased energy density from 25 Wh/l to more than 570 Wh/l, and the positive reactive current collector utilization improved from 1% to more than 60%. Also, improved capacity retention has been achieved. There has been substantial progress in realizing the key technical accomplishments, including the scalable processing.

Reviewer 2:

Although the progress to date seems modest, the reviewer commented that it is extremely good considering the difficulty in getting a solid-state battery using an iron fluoride-based cathode to work at all.

Reviewer 3:

The reviewer reported that the team demonstrated greater than 60% utilization of the cathode current collector to form active metal fluoride cathodes, which excellently meets their objective to utilize more than 50% of the cathode current collector. Ionic conductivity of the solid lithium-fluoride-based electrolyte sandwiched between the cathode and anode post-battery formation showed Li conductivity on the order of 10^{-4} S/cm, which is seven orders of magnitude higher than that of pure Li fluoride, and is also considered as good conductivity for the solid electrolytes. This result enabled the team to achieve rates in the C/2 – C/20 range, significantly higher than before. The team demonstrated energy density of more than 570 Wh/l, bringing the team closer to the goal of 1,000 Wh/l. The reviewer explained that more detailed electrochemical characterization with a graph demonstrating battery-cycle life, rate capability, impedance, etc., is desirable.

Reviewer 4:

The reviewer observed that a unique deposition system for the hybridization and fabrication of multicomponent nanolayered architectures has been designed, which has enabled the control of conductivity type and amount of transport pathways, leading to the utilization improvement of greater than 60%. Hybridization of transport pathways made the current density increase by one order of magnitude leading to the discharge rate of more than C/10. A cost-effective, scalable manufacturing process has been developed to reduce the cost. The self-formed cell stack had energy densities of greater than 500 Wh/l and 200 Wh/kg at a rate of at least C/10. Although the research team has not reached the target of a self-formed cell stack with energy densities of at least 1,000 Wh/l and 300 Wh/kg at a rate of C/10 and utilization improvement of more than 75%, they are on the right track to reach the goal. The reviewer suggested that the PI include the performance data of the battery being developed. For example, the reviewer wants to know what the ionic conductivity and electrochemical window of the Li-fluoride electrolyte are.

Reviewer 5:

The reviewer commented that the team has clearly made progress, but without knowing exactly what the team is doing, it is hard to say if this progress is fantastic or poor. If it is poor, then the reviewer said that the team has finally caught up to where everyone else is.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that it is mostly a team of one. The team appears to be making progress so the reviewer assumed some progress is a result of effective collaboration.

Reviewer 2:

The reviewer said that all the work was performed at Rutgers University.

Reviewer 3:

The reviewer commented that there are essentially no active collaborators to date, which is probably appropriate given how early and high risk this project is. The reviewer did not see this as a concern yet.

Reviewer 4:

The reviewer noted that all work has been performed at Rutgers University; the team needs to strengthen the collaborations to accomplish this project with more efficiency.

Reviewer 5:

The reviewer pointed out that the team of researchers, led by Professor Amatucci, is all located at Rutgers University and benefits from the close proximity enabling tight collaboration. Information on the team publications was not provided, making it difficult to evaluate the status of collaborative publications.

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 called the plan to improve and optimize all of the components of their battery fantastic.

Reviewer 2:

The reviewer stated that the proposed future research includes four parts, concentrating on the negative current collector, cell utilization, cell stability, and cell design, which will greatly improve the performance of the designed batteries. It is important and reasonable to continue the project. The reviewer said that the plans proposed for future research on Slide 17 are well designed and focused on the research targets. There are some specific numerical targets (described in the FY 2019 schedule) that can be judged in the future.

Reviewer 3:

The reviewer noted that the future research will be focused on achieving reversible and efficient Li-metal deposition stripping at the anode side of the battery, achieving electrochemical and mechanical stability during battery cycling, and designing and optimizing the cell architecture to achieve target parameters of energy densities of more than 1,000 Wh/l and more than 400 Wh/kg at 12 within one battery unit. The team seems to be on a good track to achieving their goals.

Reviewer 4:

The reviewer commented that to reach the proposed energy densities of more than 1,000 Wh/l and greater than 400 Wh/kg at 12V within one planar unit, the research team planned their future work in a logical manner. The team will optimize the composition and microstructure to enable high-efficiency Li stripping and plating of the negative current collector, improve the cell utilization during in situ formation of the initial amount of reactive current collector, and enhance cell stability. The proposed future work will help to achieve the final target.

Reviewer 5:

The reviewer pronounced that future work to be reasonable.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer believed that the team is working on a Li-iron fluoride system by developing a compatible solid electrolyte that prevents dendrite growth and promotes uniform Li deposition and a cathode that can be cycled. This would be a very low-cost, high-energy system if the team is successful.

Reviewer 2:

The reviewer indicated that this project focuses on self-forming thin interphases and electrodes enabling 3-D structured high-energy density batteries. The reviewer enumerated the reasons for the research strongly being consistent with DOE objectives: The weight and volume energy density targets of 350 Wh/kg and 750 Wh/l at a cell level, respectively; the necessary improvements under routine and extreme operating conditions; and achieving cost-effective methods, which is very important.

Reviewer 3:

The reviewer found that the combination of a conversion cathode and metallic Li anode addresses one of the DOE targets to achieve a high-energy density, electrochemical energy-storage system. The process of battery fabrication through a self-forming process is easy and efficient. The team utilizes low-cost materials.

Reviewer 4:

The reviewer affirmed that the project will facilitate the realization of DOE’s goals.

Reviewer 5:

The reviewer indicated that it is yet to be seen if a solid-state cell can provide the power needed for EV operation. But, the reviewer opined that it is worth pursuing given the huge advantages of solid-state cell design.

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

Reviewer 1:

All the synthesis and characterization resources for this project are sufficient, according to the reviewer.

Reviewer 2:
The reviewer said that the resources available for the team are adequate.

Reviewer 3:
The reviewer found the resources to be reasonable.

Reviewer 4:
The reviewer pointed out that no more facilities will be needed according to the previous work and proposed future research. Therefore, resources are sufficient to support the cost of raw materials, further testing, and Ph.D. students or a postdoctoral researcher.

Reviewer 5:
The reviewer suggested that the team is going to need a lot more time and money to make this system work, if it is possible at all. What they are receiving now is probably the correct amount until significant progress is made or a clear indication that progress is possible.

Presentation Number: bat326
Presentation Title: Self-Assembling and Self-Healing Rechargeable Lithium Batteries
Principal Investigator: Yet-Ming Chiang (Massachusetts Institute of Technology)

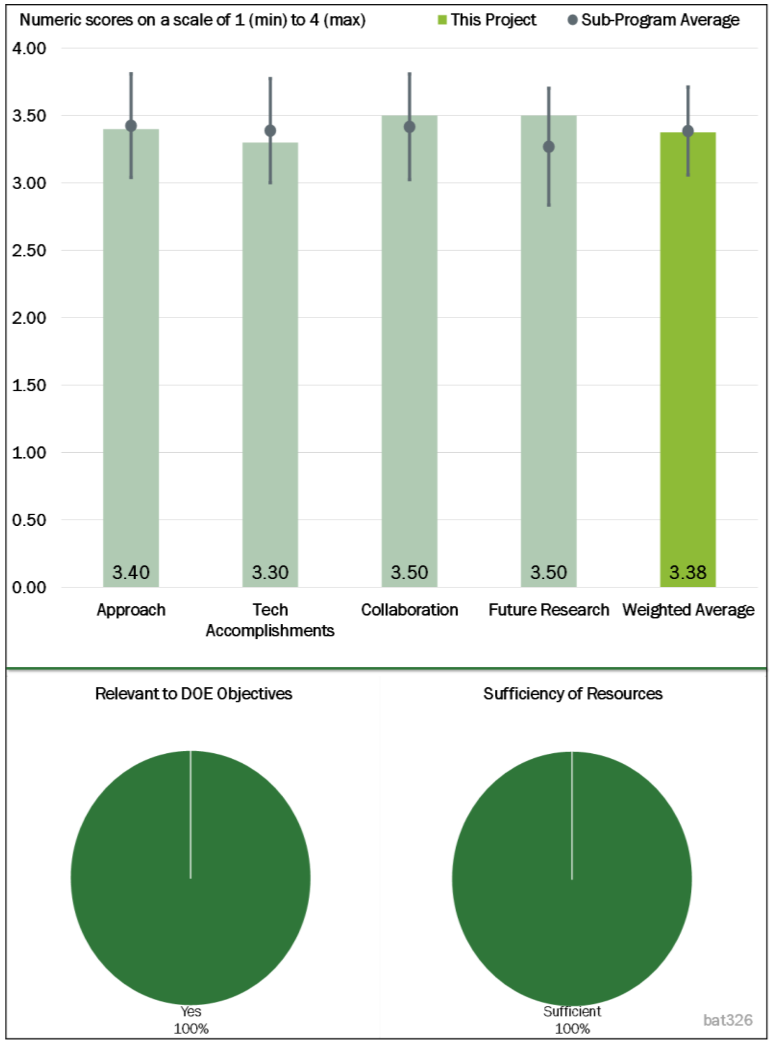

Figure 2-40 - Presentation Number: bat326 Presentation Title: Self-Assembling and Self-Healing Rechargeable Lithium Batteries Principal Investigator: Yet-Ming Chiang (Massachusetts Institute of Technology)

Presenter

Yet-Ming Chiang, Massachusetts Institute of Technology

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 and well-planned.

Reviewer 1:

The reviewer stated that the project team first performed a DFT calculation to identify and downselect self-forming and self-healing halogenated additives as it is effective to overcome most barriers. According to the DFT calculation, the team found the possibility of protecting the Li-metal anode by simply adding halogenated additives (FEC). However, according to the reviewer, the DFT calculation just declares that the decomposition reaction is reasonable in thermodynamics. Another significant aspect is whether it is reliable in dynamics. Then, the experimental matrix, which is an efficient way to explorer the influence of different parameters at the same time, was conducted and the impressive result was achieved. Besides, the battery test methods are credible to educe the result. So, the reviewer pronounced the approach to be efficient to solve the barriers.

Reviewer 2:

The reviewer said that there was a good approach to searching for testing self-forming protective layers to enable Li-metal anodes.

Reviewer 3:

The reviewer commented that the approach explored by the team is focused on discovering electrolyte formulations, including solvents, salts, and additives that would enable the formation of highly Li-ion conducting, mechanically robust, SEIs that are self-formed and exhibit self-healing properties. The additives selected belong to the class of halides and halogenated compounds, building on successful implementation of FEC. The reviewer stated that the goal is to enrich the SEI with Li fluoride to obtain a dense film and decrease the size of organic moieties in the SEI. Utilization of metallic Li as an anode protected by the formed SEI offers an opportunity to enable high-energy density batteries.

Reviewer 4:

For now, it appeared to the reviewer that adding a fluorinated solvent will yield Li fluoride on the surface. The reviewer was not sure of the value of DFT to predict this.

Reviewer 5:

In this project, the reviewer noted that theory calculation and experiments are performed to find a solution to prevent Li-dendrite formation. The team used DFT to downselect the self-forming and self-healing halogenated additives. The team used a lot of characterization tools to investigate the morphology, chemical structure, and electrochemical performance of the assembled cell to demonstrate that halide additives can effectively diminish Li-dendrite formation. According to the reviewer, it would be good to clarify why formation of a Li-fluoride layer on the anode can prevent from the formation of Li dendrites. It is better, the reviewer opined, to compare the current approach with other reported methods for the formation of Li dendrites

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

According to the reviewer, the research team has integrated theory, calculations, and experiments to select the halide additives in the electrolyte to change the morphology (less dendritic) and compactness (denser) of the deposited Li. The cycling performance of the resulting full cell is improved by the addition of fluorinated solvent into the electrolytes. Although last year's milestone has not been met yet, the progress is on track to achieve their overall objective.

Reviewer 2:

In terms of technical accomplishments, the reviewer reported that the project team had developed a new approach to measuring Coulombic efficiency (CE) that deserves further consideration. The new approach shows in the formula,

$E_{average} = 1 - Q_D/nQ_T$ where Q_D equals the total Li capacity of $Q_D = Q_T + Q_{excess}$,

Q_T equals the cycling of lithium capacity (3 mAh/cm^2 in these tests), and n equals the number of deposition/stripping cycles when there is a sudden and significant increase in (over)potential for Li stripping. The reviewer commented that the team left Q_{excess} undefined. The formula is valid for only the end of cycling when the cell is out of operation. This is forbidden in commercial use. The reviewer found that it is difficult to understand the physical significance. The formula can be written as $E_{average} = 1 - 1/n - Q_{excess}/n * 1/Q_T$, and the meaning of the subtrahend is confusing.

In respect to process, 5 of 7 quarters have been completed in 15 months with 19 months left. About half of time-consuming parts have been completed, so this reviewer commented that the project is on schedule.

Reviewer 3:

The reviewer pointed out that the team has developed a new Li-Li asymmetric cell with one Li electrode being only 20-microns thick and the other Li electrode being much thicker. Such cells enable a clear evidence for the end of the test identified by the dendritic Li plating. Moreover, the team suggested a refined way to calculate CE. Once these results are published, the reviewer recommended that the community consider adopting approaches developed by this team to become a standard way of metallic Li-anode characterization. The team demonstrated that the addition of halide additives improves morphology of the plated Li with less pronounced Li-dendrite growth compared to the cells without the additives. The cells with the additives were cycled longer than the ones without the halide additives. The reviewer observed that improved CE was demonstrated in the course of the systematic study of exploring different fluorinated solvents and additives. Although the team did not reveal the actual chemistry of the solvents and additives, the team found that di-fluorides are better than mono-fluorides, and cycling organic molecules are better than linear ones.

The reviewer indicated that the team showed an intriguing result in which the cell containing the $LiPF_6$-fluorinated solvent electrolyte (Cell 1) showed not only better stability over the course of battery cycling compared to the cell containing $LiPF_6$ ethylene carbonate-dimethyl carbonate (EC-DMC) (50/50) electrolyte (Cell 2), but also less drastic capacity fading. After 100 cycles, Cell 1 still exhibited relatively a stable 50 mAh/g, while Cell 2 showed only 10 mAh/g. The reviewer encouraged the team to analyze Li-anode post-cycling in the case of both cells. The reviewer wondered if there are islands/areas of non-dead protected Li in the case of the Cell 1, which still work well to enable this capacity. The self-healing properties of the formed SEI remained unclear to the reviewer, who encouraged the team to provide more details and characterization of the self-healing SEI.

Reviewer 4:

The reviewer remarked that the team built symmetric cells and full cells and demonstrated that there are more cycles when a fluorinated solvent is added, apparently due to the formation of lithium fluoride. Unfortunately, the reviewer opined that the CE is still way too low to be relevant.

Reviewer 5:

The reviewer found a very good improvement in the symmetric cell cycling shown, but improved cycling from 40 cycles to 70 cycles in the Li/LCO full-cell using fluoride additives. The reviewer commented that 70 cycles in a full cell is not particularly good. The Battery 500 Consortium recently showed over 200 cycles with a lean electrolyte and thin Li metal. If this poor cycling is due to poor CE, which is most likely, then the reviewer suggested that that is what needs attention. The reviewer asked if the halides improve CE, and if so, there were no data to that effect.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

According to the reviewer, the team benefits from the complementary expertise of the PI and co-PI, with Professor Chiang contributing experimental efforts and Professor Viswanathan focusing on theoretical predictions. Together, the PI and co-PI comprise a strong team. Additionally, the team collaborates with 24M Technologies, a company that is funded through an Advanced Research Projects Agency–Energy Ionics project, and the team supplies their best performing electrolytes to 24M. The reviewer noted that the team published two articles and submitted one patent application. With the results accomplished, the team should be able to demonstrate better productivity in the remaining project time.

Reviewer 2:

The reviewer said that the team has found an outside source for Li and plans on using the same source to build large cells.

Reviewer 3:

The reviewer stated that the only collaborator is 24M Technologies, which may be sufficient considering how early stage this R&D is.

Reviewer 4:

The reviewer indicated that the team has finished its collaboration with the 24M Technologies; .by receiving thin Li-metal foils, the team can do a better test.

Reviewer 5:

The reviewer remarked that the team has received thin Li-metal foils for experiments from 24M Technologies and plans to prepare and test 18 cm^2/80 cm^2 pouch cells in the future. The quality of Li-metal foils and the pouch-cell assembling technology are essential for experiments. In this project, the reviewer advised that the team needs to strengthen collaborations to accomplish this project with more efficiency.

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 remarked that the future work will be focused on overcoming the remaining barriers, which include suppressing Li-dendrite growth effectively and reproducibly, identifying new halide additives to further improve CE, fabricating the cells with greater than 10 mAh capacity, and developing Li-ion cells cycling at greater than 5 mAh/cm^2 at C/5 over 100 cycles.

Reviewer 2:

The reviewer stated that the team plans theoretical identification and quantification of better fluorinated solvents for self-formation and self-healing to improve the cycling performance and suppress the Li dendrites. The proposed research is to address the key issue of Li-metal anodes and will help to build very high energy density (more than 350 Wh/kg), rechargeable Li batteries. The team will also focus on the structural and chemical characterization of the Li-metal surface with different fluorinated solvents in the future work, which will help to establish quantitative criteria for effectiveness and reproducibility in dendrite suppression.

Reviewer 3:

According to the reviewer, the team proposed to find better fluorinated solvents for self-formation and self-healing; conduct structural and chemical characterization of Li-metal surface with different stages of cycle life; further develop an asymmetric Li-lithium cell cycling methodology to resolve CE at different stages of cycle life; demonstrate Li-Li asymmetric cells that meet established criteria cycling at $\geq$ 3 mAh/cm^2 at C/5 rate over 30 cycles; and operate Li-NMC full cells with high areal capacity of more than 3 mAh/cm^2 for more than 100 cycles.

The reviewer proposed that further study on better fluorinated solvents and the relative structural and chemical evolution on the Li-metal surface are very much necessary to understand the mechanism of fluorinated solvents. To commercialize this research, the reviewer said that higher areal capacity of $\geq$3 mAh/cm^2 Li-NMC full cells is the first step, and achieving the asymmetric Li-lithium cell $\geq$3 m h/cm^2 is the first efficient method. However, the concentration of fluorinated solvents is also a notable problem to understand the influence of fluorinated solvents.

Reviewer 4:

The reviewer commented that the team plans to use DFT to discover additional solvents. It was not clear to the reviewer as to what properties the team would like the SEI to have other than Li fluoride.

Reviewer 5:

The reviewer said if the poor full cell cycling is due to low CE, then that is what needs attention. The reviewer asked if the halides improve CE, as there were no data about that.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer commented that the purpose of this project is to suppress the dendrite growth on the surface of Li-metal, enabling a very high energy density (greater than 350 Wh/kg), rechargeable Li battery to improve the driving range and reduce the cost for electric vehicles. This project meets the mission of DOE to ensure America's prosperity by addressing its energy at this point. A Li-metal anode is a promising anode material with ultrahigh energy density and low potential. According to the reviewer, the lower the potential anode is, the higher voltage full cells are and the higher power density full cells are. A Li-metal anode is one of a few materials that show high specific capacity and low potential in the same time. However, the reviewer pointed out that the emergent issue is to solve the safety problem that arises from the dendrite growth on the surface of Li-metal. Therefore, the project supports the overall DOE objectives.

Reviewer 2:

The reviewer remarked that the project explores the protective properties of Li-halide films on Li-metal anodes and aims at demonstrating self-assembling/self-healing batteries. In addition to developing a simple and scalable self-forming battery fabrication process, utilizing metallic Li as an anode offers an opportunity to reach high energy density (greater than 350 Wh/kg), which is sought for powering EVs and making EVs a more affordable means of transportation. The reviewer agreed that these goals are in line with the DOE targets.

Reviewer 3:

The reviewer affirmed that the self-formed Li-halide based solid-electrolyte interface could improve the cyclic performance of batteries and extend the lifetime of batteries.

Reviewer 4:

The reviewer opined that trying to get Li to work is consistent with trying to get to higher energy density.

Reviewer 5:

The reviewer stated that enabling Li-metal anodes is clearly very relevant.

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

Reviewer 1:

The reviewer noted that the project team mainly explored electrochemical formation of Li-halide based solid-electrolyte interfaces. The funding for 2018 is $462,912. The reviewer pointed out that no more facilities will be needed according to the previous work and proposed future research. Therefore, resources are sufficient to support the cost of raw materials, further testing, and Ph.D. students or a postdoctoral researcher.

Reviewer 2:

All the characterization, synthesis and theory calculation tools are sufficient to meet the milestone proposed in this project in time, according to the reviewer.

Reviewer 3:

The reviewer said that the resources are sufficient for this effort.

Reviewer 4:

The reviewer found the funding to be reasonable for this project.

Reviewer 5:

The reviewer commented that the resources available for the team are adequate.

Presentation Number: bat328
Presentation Title: Dendrite-Growth Morphology Modeling in Liquid and Solid Electrolytes
Principal Investigator: Yue Qi (Michigan State University)

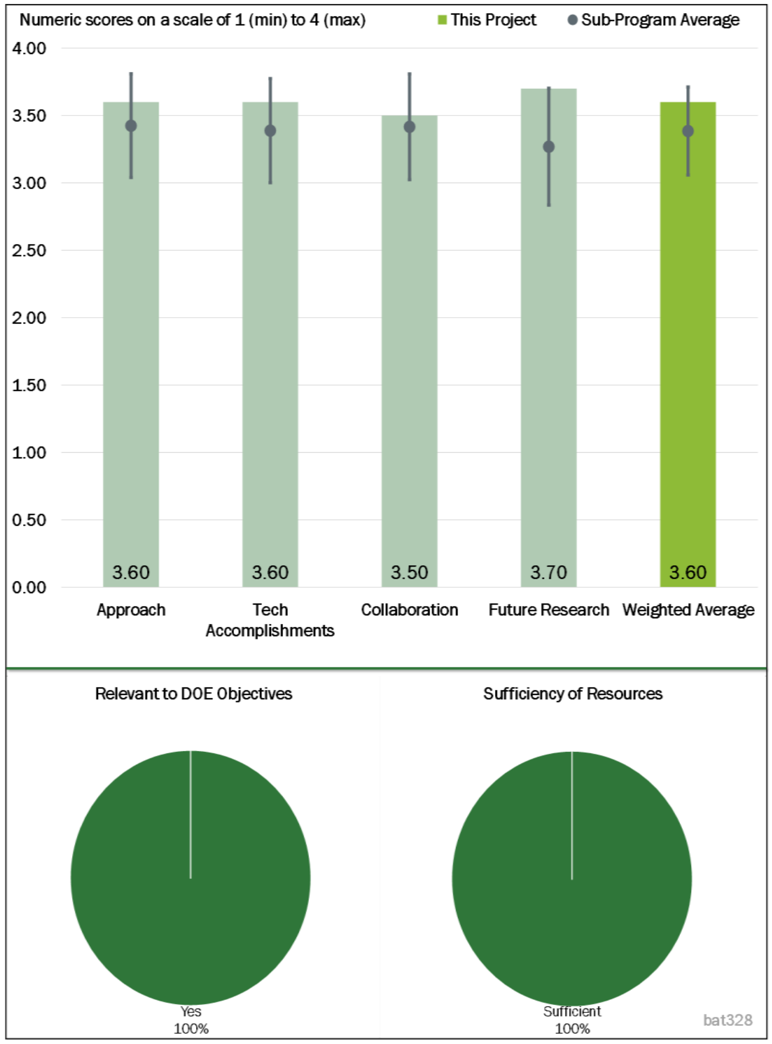

Figure 2-41 - Presentation Number: bat328 Presentation Title: Dendrite-Growth Morphology Modeling in Liquid and Solid Electrolytes Principal Investigator: Yue Qi (Michigan State University)

Presenter
Yue Qi, Michigan State University

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 and well-planned.

Reviewer 1:
The reviewer said that this project utilizes a multiscale modeling and experimental approach, including a combination of micron-scale and atomic-scale modeling that is used to predict Li-dendrite nucleation and growth kinetics and morphology; the theoretical predictions are validated through experimental investigations. The results from this project, according to the reviewer, can help to accelerate the adoption of Li-metal electrodes in current and emerging battery technologies. In parallel, new computational models suitable for the computational characterization of Li-metal anode and solid-electrolyte interface have been developed and potentially can be universally applied to other meta-anode systems.

Reviewer 2:
The reviewer liked the methodical approach of going after this problem from many angles.

Reviewer 3:
The reviewer commented that this was a good approach to trying to uncover more clues about the growth of dendrites in both solid- and liquid-electrolyte cells.

Reviewer 4:
The reviewer stated that the project aims to simulate Li-dendrite evolution on the Li-metal anode side through multiscale modeling and an experimental approach along with micron-scale, phase-field models and atomic-scale, DFT-based simulations. The reviewer said that the modeling could be used to predict the Li-dendrite nucleation, growth kinetics, and morphology. The project used microscale experiments to observe the morphology of dendrites. The project is well designed and feasible.

The reviewer wondered whether the model to be developed will predict the critical factors that govern the nucleation and growth of Li dendrites. According to the reviewer, the PIs need to clarify what the criteria are for designing the surface coating on the Li-metal anode that can suppress the Li-dendrite formation.

Reviewer 5:

The reviewer indicated that the project led by Professor Yue Qi focuses on dendrite-growth morphology modeling in liquid and solid electrolytes. An efficient model was carried out to design the desired properties of artificial SEI coatings, the microstructure of solid-electrolyte materials, and the corresponding battery-operating conditions to avoid dendrite growth during cycling. The reviewer characterized this project as having clear and viable research thoughts, which can provide further directions on designing durable and safe Li-anodes for high-energy density Li-rechargeable batteries.

However, the reviewer offered some comments on the approach of this project for consideration: Because the model plays a crucial role on the calculation results, it is important to know whether the selected models in liquid and solid electrolytes are reasonable for practical cells. The reviewer wanted to see a discussion of more application conditions. In addition, correlations between the calculated results and experimental results should be discussed as well as performing more experiments to confirm the results from models. The reviewer pointed out that the electrolyte also plays an important role in batteries and wanted to know more about the influence of different electrolytes on Li dendrites in the models. The reviewer asked what the biggest differences are on the dendrite-growth of Li anodes in liquid and solid electrolytes and the reasons that lead to this difference. For further practical applications based on understanding from the model, the reviewer suggested that more full cells and punch cells should be assembled for high-energy density Li-rechargeable batteries to meet the DOE target. Lastly, the reviewer asked to see a detailed budget for every year in order to decide whether the remaining funds can support further research.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented than an implicit multiscale dendrite-growth model has been developed, which shows that lowering the exchange current (I_0) is the most efficient method of Li-plating to achieve a smooth surface and experimentally tunes the I_0 via surface engineering. A new, explicit model was also constructed to simulate Li-dendrite formation and growth in solid electrolytes with microstructure and internal defects (pores). The team is now on the right track to develop a multiscale model to predict the evolution of Li-dendrite morphology.

Reviewer 2:

The reviewer found that there was very nice insight into the effect of I_0 on dendrite growth with experimental results presented to confirm those predictions.

Reviewer 3:

The reviewer noted that significant progress in many areas has been made.

Reviewer 4:

In this project report, the reviewer remarked that the current accomplishments of the project are interesting and important. In detail, an implicit multiscale dendrite growth model was developed to investigate Li plating under different conditions. In addition, a new, explicit model was constructed to simulate Li-dendrite formation and growth in solid electrolytes with microstructure and internal defects. The reviewer posited that this in-depth understanding can give further insight into Li-dendrite formation and growth and provides good directions on the design of Li anodes. But, the reviewer cautioned that the completed percentage is only 35%, and during the ongoing project, more complex models will take longer time. The reviewer questioned whether the goals of this project can be finished when the project reaches the deadline and asked for some strategies to be provided to make sure of the successful completion of this project.

Reviewer 5:

The reviewer summarized the project results by saying that theoretical models that could be used to compute charge transfer reactions, calculate energy barriers, and predict metal dendrites formation have been developed and successfully used. The energy barriers of Li-ion desolvation and Li-ion diffusion through the solid electrolyte interface were calculated and shown to vary with potential. The morphology of Li dendrites under varying electrochemical conditions was predicted and compared to the morphology of magnesium dendrites. The team showed that lowering the exchange current can lead to suppressed Li-dendrite growth. A coating was applied on the Li surface; however, so far no improvements have been shown. Li-mossy structures grew and cracks in coatings were observed. Lastly, ALD of a LiPON coating showed the potential to prevent metallic-Li nucleation.

The reviewer questioned the fact that, in the team's report, only two papers are shown as published, and three manuscripts submitted. With such a strong team, the reviewer said it is desirable to see more products. The reviewer queried whether controlling current density during battery operation, as suggested, is the most efficient way to control Li-dendrite formation. The reviewer pointed out that this is not practical for real battery operation. The reviewer said it is desirable to see more practical ways to suppress Li-dendrite growth. The researchers plan to investigate the effect of coatings and electrolyte additives, which can provide acceptable, practical ways to minimize or ideally eliminate formation of lithium dendrites.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that Yue Qi leads the project. The PI has established collaborations and coordination with other institutions. For example, Gary Rubloff from the University of Maryland applied an ALD LiPON coating, which has higher Li conductivity compared to typical SEI components. Katherine Jungjohann from SNL Albuquerque investigated the Li morphology using a sealed liquid cell for in situ STEM, and investigated the effects of artificial SEI coatings on morphology at nanometer scale. Yan Yao from the University of Houston compared Li and magnesium plating morphology. Jie Xiao from PNNL and the University of Arkansas investigated the effect of electrolyte additives and their role on SEI. These collaborators provided in-depth insights using experimental tests, which can further confirm and support the calculation results. The reviewer confirmed that this is very important to successfully complete this project.

Reviewer 2:

The reviewer stated that this project is performed through collaborations with the University of Maryland, SNL Albuquerque, the University of Houston and PNNL, and the University of Arkansas. The reviewer found the he collaborations to be very effective.

Reviewer 3:

The reviewer remarked that the project appears to make relationships and obtain assistance in critical areas where it is needed.

Reviewer 4:

The reviewer indicated that the team is led by Professor Qi, a leading computational scientist, who focuses on atomic simulations. Other members include Professor Chen, who contributes microstructure modeling, and Dr. Xiao and Dr. Lu, who provides experimental results on Li-dendrite formation. Other collaborators are Professor Rubloff (coatings using ALD), Dr. Jungjohann (in situ STEM), Professor Yao (experimental comparison of Li and magnesium plating morphology), and Professor Xiao (the effect of electrolyte additives and their role in SEI). Overall, this is a very strong team with complementary expertise covering all relevant areas, including both computational and experimental research. The reviewer indicated that it would be desirable though to see more collaborative publications from such a strong team.

Reviewer 5:

The reviewer viewed that it is fairly early in this R&D project to be too concerned about collaboration. The team has the expertise and facilities it needs.

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:

According to the reviewer, the proposed future research will be focused on modeling of the SEI and correlation of SEI properties with Li-dendrite morphology in a liquid electrolyte. Furthermore, electrochemical-mechanical-structural coupling effects in cells with solid electrolytes will be investigated to propose a mechanism of Li-dendrite formation. Theoretical predictions will be verified through experiments.

Reviewer 2:

The reviewer found the future work to be well conceived.

Reviewer 3:

The reviewer commented that, to gain full understanding of the SEI and Li-dendrite growth, the project will further correlate SEI properties with Li-dendrite morphology in a liquid electrolyte and capture the internal structures of SEI. The future work is logically planned, according to the reviewer. Through the modeling and experiments, jointly designed effective combinations of bulk solid electrolyte and surface coatings will improve the cycling efficiency and life of lithium-rechargeable batteries.

Reviewer 4:

The reviewer said that all future work looks relevant and well-focused. The reviewer was curious about where some of these parameters are coming from and asked if they can reproduce existing data, e.g., the current at which the transition occurs from mossy Li deposition to dendritic Li deposition. The reviewer encouraged the team to engage with the Battery 500 Consortium R&D teams.

Reviewer 5:

In this project report, the reviewer summarized some of the proposed future research as follows: Correlate SEI properties with Li-dendrite morphology in a liquid electrolyte; develop an explicit SEI dendrite-growth model to capture the internal structures of SEI; investigate the electrochemical-mechanical-structural coupling effects and explore the mechanism of Li-dendrite formation in solid electrolytes from a phase-field model; and modeling and experiments jointly designed in effective combinations to improve the cycling efficiency and life of Li-rechargeable batteries. The reviewer opined that this future research is highly desirable to give further directions for the design of highly durable and safe Li anodes. However, the reviewer asked for more details and possible risks to be provided and discussed rather than only the goals for every challenging research topic.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer noted that the project led by Professor Yue Qi focuses dendrite-growth morphology modeling in liquid and solid electrolytes to solve the issues of dendrite growth, low CE, short calendar, and cycle life in Li-metal film electrodes. The reviewer posited that the successful accomplishment of this project can enable the design of durable and safe Li anodes for high-energy density, Li rechargeable batteries that can meet the DOE target for EV applications of greater than 350 Wh/kg and less than $100/kWh use.

Reviewer 2:
The reviewer stated that this research addresses a challenge of developing high-energy density batteries utilizing a Li-metal anode, which is one of the DOE targets. Such batteries, if they meet safety and cost requirements, are attractive for application in EVs.

Reviewer 3:
The researcher affirmed that the research will provide an interesting modeling approach to understand Li-dendrite growth during cycling, which will accelerate the adoption of Li-metal electrodes in current and emerging battery technologies.

Reviewer 4:
The reviewer commented that understanding the mechanism for Li-dendrite growth is the key to stopping it.

Reviewer 5:
The reviewer stated that R&D into Li-metal anodes is highly relevant.

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

Reviewer 1:
The reviewer pronounced the resources for modeling, synthesis, and characterization for experiments to be sufficient to achieve the proposed project goals.

Reviewer 2:
The reviewer said that the resources available for the team are adequate.

Reviewer 3:
The reviewer remarked that this is a well-managed project.

Reviewer 4:
The reviewer had no issue with resources.

Reviewer 5:
The reviewer praised the leader of this project for having good collaborations and coordination with other institutions. These collaborations can greatly support the successful accomplishment of this project. But, the reviewer wanted to see some other sources of technical personnel and facilities to support this project. Ph.D. students and postdoctoral researchers should focus on this project in order to achieve successful accomplishment within the given time. In addition, more sources should be required to realize fast and exact computational simulations.

Presentation Number: bat329
Presentation Title: Understanding and Strategies for Controlled Interfacial Phenomena in Lithium-Ion Batteries and Beyond
Principal Investigator: Perla Balbuena (Texas A&M University)

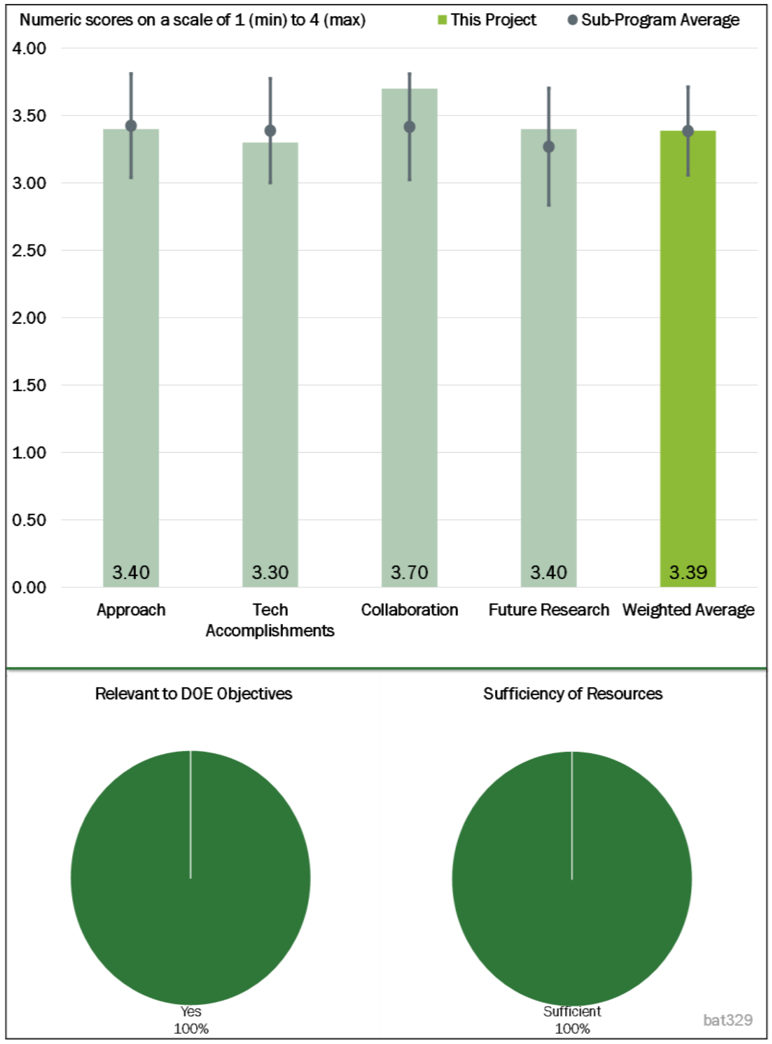

Figure 2-42 - Presentation Number: bat329 Presentation Title: Understanding and Strategies for Controlled Interfacial Phenomena in Lithium-Ion Batteries and Beyond Principal Investigator: Perla Balbuena (Texas A&M University)

Presenter

Perla Balbuena, Texas A&M University

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 and well-planned.

Reviewer 1:

The reviewer commented that the project utilizes a multiscale modeling approach to elucidate parameters that impede extending the lifetimes of the Si and Li anodes. The project addresses such aspects as SEI formation, cracking of Si particles, and growth of Li dendrites. All findings obtained through theoretical predictions are compared with experimental results.

Reviewer 2:

The reviewer said that the project was a very nice and very challenging approach to investigating the character and structure of Li-metal and Si SEIs.

Reviewer 3:

The reviewer pronounced the project as an excellent, first-principles approach.

Reviewer 4:

The reviewer remarked that the project aims to address the interfacial issues that affect the lifetimes of the Si and Li-metal anodes by synergistic multiscale modeling. The modeling included the electronic structure and dynamics, the atomistic classical molecular dynamics, and the mesoscopic modeling. The modeling result is compared with the experimental evidence. The reviewer wondered if the modeling can predict the critical factors that form Li dendrites. The reviewer posited that it would be good if the calculation and simulation can predict and evaluate Li-dendrite nucleation and growth.

Reviewer 5:

In this project, the reviewer noted that synergistic multiscale modeling (ab initio, classical molecular dynamics, and mesoscopic level models), first-principles approach, and many other theoretical calculation approaches are applied to explore interfacial problems, such as SEI growth, Si-particle cracking due to volume expansion, Li-dendrite formation to address the barriers of loss of available capacity, and materials degradation during cycling and lifetime of the cell. These approaches can reveal the mechanism of the interfacial problems to a certain degree, and the reviewer suggested that the authors should consider whether the selected models in liquid electrolytes are reasonable for practical cells. Thus, more application conditions should be included. On the other hand, based on the calculation results, the reviewer proposed that more specific experimental strategies should be designed and provided to develop high-performance Si-/Li-anode materials, which will be more helpful to meet the targets.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that calculation and simulation results have identified the chemical origin of dendrite formation, the critical issue that leads to the loss of available capacity. The team elucidated the passivation role of the SEI layer on Li-metal. The team has completed the milestone. The result of SEI growth and multiscale characterization of dendrite growth are very interesting. Test and analysis of coatings for mitigation of dendrite growth are going on.

Reviewer 2:

The reviewer asserted that the project was a careful assessment of the relative rates of reduction of Li^+ in the presence of Li-metal as compared to other compounds that can compete for the electrons. It was also an investigation of preferential dendrite conditions.

Reviewer 3:

The reviewer praised the progress on Li-metal SEI and dendrite growth as good.

Reviewer 4:

The reviewer found intriguing computational results that showed differences for various electrolyte compositions in preferential reduction of Li or an electrolyte solvent molecule on the surface of a Li-metal anode. Additionally, the role of defects on the Li surface and the coating of the Li surface with molecules, typically found in SEI, towards Li reduction has been elucidated. These results are crucial for the understanding of Li-dendrite growth and developing ways to suppress Li-dendrite formation. The reviewer noted that modeling approaches have been developed to predict SEI growth and evolution, and a mesoscopic model of Li-dendrite growth revealed experimental conditions of electrochemical cycling that lead to different morphology of the plated Li. High overpotentials caused by high applied currents were found to promote Li-dendrite growth. The role of the Li-surface coating is being investigated through combined computational and microscopy characterization.

While this report contains multiple interesting results, it remained unclear to the reviewer what guidelines the computational approaches delivered for the experimental scientists. There were no explicit conclusions on the specific experimental parameters and how they need to be controlled to suppress Li-dendrite formation, mitigate the effect of Si cracking, or form the SEI that would lead to improved battery performance. The reviewer encouraged the team to state their conclusions and suggestions to the experimental scientists more clearly. The reviewer wanted to know the best Li surface, the best coatings (chemistry, thickness), the electrolyte formulations, and so on.

Reviewer 5:

In this project, the reviewer commented that technical accomplishments, such as identifying chemical origin of dendrite formation; elucidating the passivation role of SEI layer on Li-metal; initial studies of SEI growth; multiscale characterization of dendrite growth; and test and analysis of coatings for mitigation of dendrite growth on Li-metal have been realized. Some research papers have been published, which can give further insights into Li-dendrite formation and growth and provide good directions on the design of Li anodes.

However, the reviewer encouraged the team to consider more complex models, even knowing that this will take a longer time. Thus, the reviewer suggested that the authors should give a more detailed schedule to carry the program forward to finish on time. Additionally, these technical accomplishments are limited to theoretical calculations, and accomplishments on specific experimental strategies are lacking. Especially noteworthy is that there has been slow progress of research on a Si anode

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

In this project, the reviewer stated that there are many collaborations and coordination with other institutions. Contributors to a large part of the reported work are Professor Jorge Seminario, a co-PI from Texas A&M University (prime) on classical molecular dynamics (MD) and Professor Partha Mukherjee, a co-PI from Purdue University (sub-awardee on mesoscopic modeling). Y. Horowitz, Hui-Ling Han, and Gabor Somorjai from UCB contributed in the area of sum frequency generation vibrational spectroscopy together with ab-initio molecular dynamics simulations from Texas A&M University to characterize SEI formation at the surface of amorphous Si anodes. M. Vijayakumar from PNNL did experimental work while Texas A&M University did the theoretical characterization of electrolyte reduction over Li-metal surfaces covered by selected SEI components. Professor Shahbazian-Yassar from the University of Illinois at Chicago examined graphene-oxide coated materials as protection for copper current collectors where Li is plated along with characterization of surface science techniques of surface changes and reactions and DFT and ab-initio molecular dynamics simulations from Texas A&M University.

The reviewer pointed out that the work of these institutions is also clearly divided: synergistic multiscale modeling approach at Texas A&M University and Purdue University, SEI formation on amorphous Si surfaces at University of California at Berkeley, the effect of current collector coatings on dendrite formation at University of California at Berkeley, and the passivation role of SEI at PNNL., The reviewer asserted that these collaborators are well coordinated, which is very important to successfully complete this project.

Reviewer 2:

Professor Balbuena, a computational scientist, leads the team. Other members include Professor Seminario, who contributes classical MD simulations, and Professor Mukherjee, who provides mesoscopic modeling. Other collaborators are researchers from UCB (vibrational spectroscopy characterization to characterize SEI formation at the surface of Si anodes), researchers from PNNL (experimental characterization of electrolyte reduction over Li-metal surfaces), and researchers from the University of Illinois at Chicago (experimental microscopy characterization). Overall, the reviewer found that this is a strong team with complementary expertise covering all relevant areas, including both computational and experimental research. The team is extremely productive with both individual PI (or co-PI) and collaborative publications. The total number of the reported published papers is 11, which is very high.

Reviewer 3:

The reviewer found the team to be well organized; and the work done by the team member is complementary to each other.

Reviewer 4:

According to the reviewer, many researchers with different skills contributed to this effort.

Reviewer 5:

The reviewer was glad that this team is working with PNNL to confirm its theoretical predictions with experimental data.

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

Reviewer 1:
The reviewer remarked that the future work largely focuses on understanding the effect of electrolyte composition on Li-dendrite formation, Si cracking, and SEI formation. The team will explore Li plating in the presence of K^+ and Na^+ ions as well as the effect of operating conditions (temperature and current rate).

Reviewer 2:
The reviewer said that the team will focus on developing the strategies for controlling the deposition effect on Li-metal and for enhancing the practical utilization of Si anodes.

Reviewer 3:
The reviewer pronounced the work to be very good and noted that relevant future work is planned.

Reviewer 4:
In this project, the reviewer pointed out that further plans have been provided to characterize Li^+ electrodeposition in the presence of other ions (Na^+, K^+) and study the effects of operating conditions (temperature and C-rate on dendrite formation). Macroscopic effects during cycling of Si and Li anodes will be looked at along with identifying electrolyte or electrode additives that may help mitigate the just-discovered chemical effects in Li-metal anodes. Other work involves identifying electrolyte additives or other strategies for Si anodes and developing alternative charging strategies for Li-metal anodes. These plans correspond to the accomplishments and projects goals, but the reviewer found these plans not to be specific enough. The reviewer asked for more details along with considering possible problems and solutions to demonstrate their feasibility.

Reviewer 5:
The reviewer was not sure why the team is planning on investigating Na^+ or K^+. The reviewer liked the idea of determining the effect of C-rate and why dendrites form before mass transfer limits are reached. The reviewer expressed doubt about what a macroscopic effect is with regard to plating. The reviewer appreciated the idea that now that we understand Li-dendrite formation, we need to do something to prevent it. The reviewer did not think that charging strategies are the answer, but who knows.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer stated that this project focuses on evaluating and characterizing interfacial phenomena in lithiated Si and Li-metal anodes; the project also develops strategies leading to controlled reactivity at electrode/electrolyte interfaces using advanced modeling techniques based on first principles, which is crucial for controlling ICL and improving lifetimes. Therefore, the reviewer said that the research approaches in this project are consistent with DOE objectives.

Reviewer 2:
The reviewer affirmed that, if successful, the calculation and simulation will provide insight into the stability of the anode/electrolyte interface.

Reviewer 3:
The reviewer commented that understanding of the SEI formation and mechanical stability of SEI on Si anodes and SEI formation, as well as Li-dendrite growth on Li anodes, which are the focus of this project, are crucial to enable high-energy density Li-ion or Li-sulfur batteries with minimized ICL and maximized lifetimes. Thus,

the reviewer opined that this research is highly relevant to the DOE target of developing next-generation batteries for EV applications.

Reviewer 4:
The reviewer found the work to be very relevant to DOE objective of getting to higher energy densities.

Reviewer 5:
Working on Li-metal anodes is highly relevant, according to the reviewer

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

Reviewer 1:
The reviewer was enthusiastic about the fantastic progress the PI was making with the present resources.

Reviewer 2:
The reviewer asserted that the resources and equipment are sufficient to implement the project.

Reviewer 3:
The resources available for the team are adequate, according to the reviewer.

Reviewer 4:
The reviewer had no issues with resources.

Reviewer 5:
The reviewer remarked that the group and cooperative institutions in this project are proficient in theoretical calculation and many high-level research papers have been published. In consideration of the research cost, the expenditure in this project is abundant theoretically. Therefore, the group possesses sufficient resources for equipment and researchers to finish the objectives. However, the reviewer pointed out that nearly two-thirds of the time has passed but only 40% of the project has been finished. Therefore, the reviewer urged that the progress should be accelerated.

Presentation Number: bat330
Presentation Title: Electrochemically Responsive, Self-Formed, Lithium-Ion Conductors for High-Performance Lithium-Metal Anodes
Principal Investigator: Donghai Wang (Penn State University)

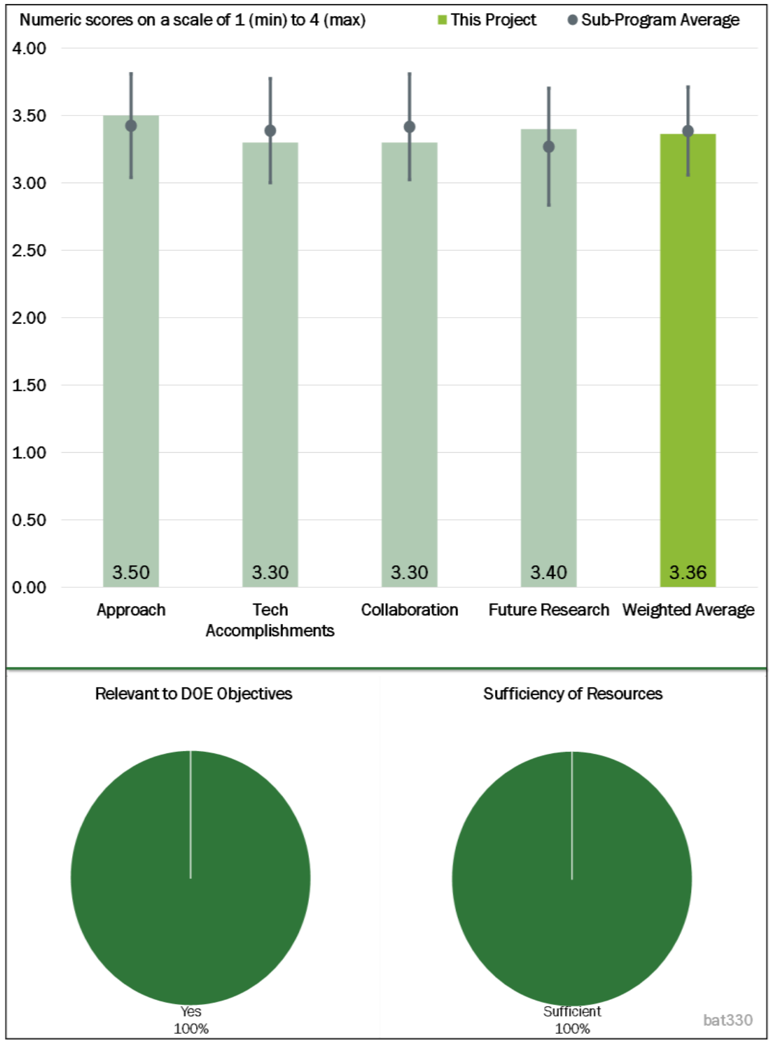

Figure 2-43 - Presentation Number: bat330 Presentation Title: Electrochemically Responsive, Self-Formed, Lithium-Ion Conductors for High-Performance Lithium-Metal Anodes Principal Investigator: Donghai Wang (Penn State University)

Presenter

Donghai Wang, Penn State University

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 and well-planned.

Reviewer 1:

The reviewer complimented that the approach based on using a strategy that stabilizes the Li-metal–liquid electrolyte interface by coating the Li-metal surface with multiphase inorganic-organic hybrid ion conductors with tunable multifunctional organic components and controlled inorganic components is quite novel and is well planned. The approach using the different phases seeks to use a SEI with properties for conduction as well as good Li-metal deposition.

Reviewer 2:

The approach is logical and well designed to address one of the major issues confronting the development of a Li-S battery—polysulfide shuttling and an unstable Li/electrolyte interface. To address these issues, the team has a comprehensive plan to develop a self-formed Li-ion conductor as a protective layer for Li-metal anodes. This will in theory enable Li-metal anodes to cycle with a high efficiency. The reviewer found that this a good idea and the PI has laid out a well-designed plan and a realistic time schedule.

Reviewer 3:

The reviewer observed a good concept and approach to try and design multiphase inorganic-organic hybrid ion conductors with tunable multifunctional organic components and controlled inorganic components for Li-metal anodes.

Reviewer 4:

The reviewer commented that many researchers have suggested some type of hybrid approach where a combination of tough inorganic material and soft, polymer forming material are combined to stop dendrites. The project team makes an attempt at this approach.

Reviewer 5:

The reviewer noted that in this project, the team explored new organic Li-and-sulfur-containing additives to form Li-conducting SEI on the surface of a metallic Li anode to enable robust protection and lead to the Li-S batteries with high energy density. The team aim to reaching a goal of Li dendrite-free cycling and CE of greater than 99.7%.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that excellent progress has been achieved this past year. The team was able to demonstrate that organo-Li_xS_y Li protection layers can effectively suppress dendrite growth and significantly improve the cycling efficiency. The team also investigated new cathodes that enable high-sulfur mass loading and a low electrolyte/sulfur ratio.

Reviewer 2:

The reviewer said that improvement in cycling stability is quite good although the CE is still stuck near 99%, which means a full cell cycle life of only 220 cycles if we start with triple the Li excess. The reviewer commented that a much higher CE is clearly needed, which is a real challenge with Li-metal anodes. The reviewer pointed out that these coatings do help CE and impedance rise, which is good.

Reviewer 3:

The reviewer pointed out that the Li in the cell with the second-generation electrolyte appears smoother than with the first-generation electrolyte, and that the XPS shows C-fluoride compounds. The data appear to suggest that there are more organo-sulfides present in the SEI with the second-generation electrolyte and less C-fluoride compounds. The reviewer said the modulus of the SEI appears to decrease with the second-generation, but the reviewer was unable to tell if this is a good or bad thing. The reviewer remarked that the project team obtained more cycles with the new electrolyte and show higher cycling efficiency based on plating and stripping on copper, but all three are around, 99% which is too low for a practical cell. The reviewer said that there is no increase in impedance when switching to the second-generation electrolyte. The reviewer did not understand what the project team is measuring when removing all of the Li from the copper and then performing electrochemical impedance spectroscopy (EIS). The retained capacity is better in a full cell with sulfur as the cathode but no explanation as to why. The reviewer said that the project team does not indicate how much excess Li is used in the cell for full cycling.

Reviewer 4:

The reviewer acknowledged that while significant progress has been made on the coating, the reported CE is not good enough. The PI has not yet shown that that it can be compatible with Li-S system required conditions including mass loading and E/S ratio.

Reviewer 5:

The reviewer commented that the second-generation organo-Li_xS_y additive molecules to be used in electrolytes for metallic Li protection were developed. In comparison to the first-generation linear molecules, the second-generation molecules are cyclic. The reviewer said that the addition of the second-generation additives into the electrolyte showed improved Li anode morphology after 100 cycles, and that Li dendrite growth is partially suppressed. The reviewer remarked that the project team demonstrated a CE of ~99.1% at a current density of 2 mA/cm^2 and capacity of 1 mAh/cm^2, bringing the team closer to its target of 99.7% CE.

The reviewer desired a better explanation about differences between the sulfur-and-Li-containing SEI layer on the surface of the Li anode and reduction of polysulfides dissolved in the electrolyte and related to the shuttle effect. The reviewer asked does Li_2S and Li_2S_2 form in the course of the reduction of the sulfur-and-Li-containing developed organic additives, and how the formed SEI interacts with the polysulfides dissolved in the electrolyte. Additionally, the reviewer desired more results and a better understanding of the effect of the formed Li-and-sulfur-containing SEI on the metallic Li surface. The reviewer pointed out that the team plans to investigate it in the future.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said that the PI has good collaborations for theory and Li-S batteries.

Reviewer 2:
The reviewer was glad to see the team is collaborating with PNNL on making full cells and not trying to figure this out on their own.

Reviewer 3:
The reviewer noted that Prof. Wang at Pennsylvania State University (PSU) leads the project. The collaborators include Prof. Kim (atomic force microscopy characterization) and Prof. Chen (modeling of Li dendrite growth) at PSU and Dr. Liu (fabrication of Li-S batteries) at PNNL. The team is highly productive with five articles, including collaborative articles, published in 2017-2018.

Reviewer 4:
The reviewer commented good collaboration with PSU colleagues as well as with PNNL.

Reviewer 5:
The reviewer observed reasonable collaborations at this stage of the project.

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

Reviewer 1:
The reviewer remarked that future work is to continue similar development, and that results on Li-metal/sulfur cells are quite promising.

Reviewer 2:
The reviewer remarked that the team is proposing work that is both logical and necessary to move forward. The reviewer said that a new, hybrid organo-Li_xS_y/organo-Li_xPyS_z composite will be developed.

Reviewer 3:
The reviewer detailed that the future work will explore properties of the Li-and-sulfur-containing SEI formed on the surface of a Li anode to suppress growth of Li dendrites in the course of Li-S battery cycling. The team will develop new electrolyte additives with the goal to reach the target CE of 99.2%. Further, the team will develop an inorganic/organic composite protection layer utilizing best-performing organic molecules to reach the CE of 99.7%.

Reviewer 4:
The reviewer pointed that out that future plans are to optimize everything. The reviewer said that there is no indication in these slides how the team plans to optimize the chemistry other than through trial and error, nor is there any reason to believe that through trial and error with the present chemistry the team will achieve much better CE.

Reviewer 5:
The reviewer remarked that the PIs have a reasonable plan to increase the performance of their coating, but little detail was given about how this to be achieved other than using a second-generation coating.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer pointed out that Li anode protection is a high priority for the DOE objectives because of a need to find higher energy density anodes.

Reviewer 2:

The reviewer said that this project is highly relevant and supports DOE/VTO goals. It aims to develop a new Li-ion conductor that will enable high-performance Li-metal anodes. Li-metal anodes can lead to a 50% increase in the energy density of conventional Li-ion batteries with Li-metal oxide cathodes.

Reviewer 3:

The reviewer said that it is highly relevant to work on stabilizing the Li-metal interface.

Reviewer 4:

The reviewer said that developing protective layers for Li-metal does support DOE's overall objective of improving energy density because it allows going from Gr to Li, which has ten times the capacity for Li per gram of material.

Reviewer 5:

The reviewer said that protection of a metallic Li anode through the formation of a Li-conducting SEI layer with specific chemical composition enabled by the developed Li-and-sulfur-containing new organic molecule electrolyte additives can enable Li-S batteries with high energy density, which is one of the DOE's targets for the next-generation EV applications.

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 resources are sufficient.

Reviewer 2:

The reviewer said that the team has sufficient resources for successful completion of the mission in a timely manner.

Reviewer 3:

The reviewer found that for this trial and error approach, this is enough resources.

Reviewer 4:

The reviewer said that the resources available for the team are adequate.

Reviewer 5:

The reviewer observed good resources.

Presentation Number: bat332
Presentation Title: High Electrode Loading Electric Vehicle Cell
Principal Investigator: Mohamed Taggougui (24M Technologies)

Presenter

Mohamed Taggougui, 24M Technologies

Reviewer Sample Size

A total of four reviewers evaluated this project.

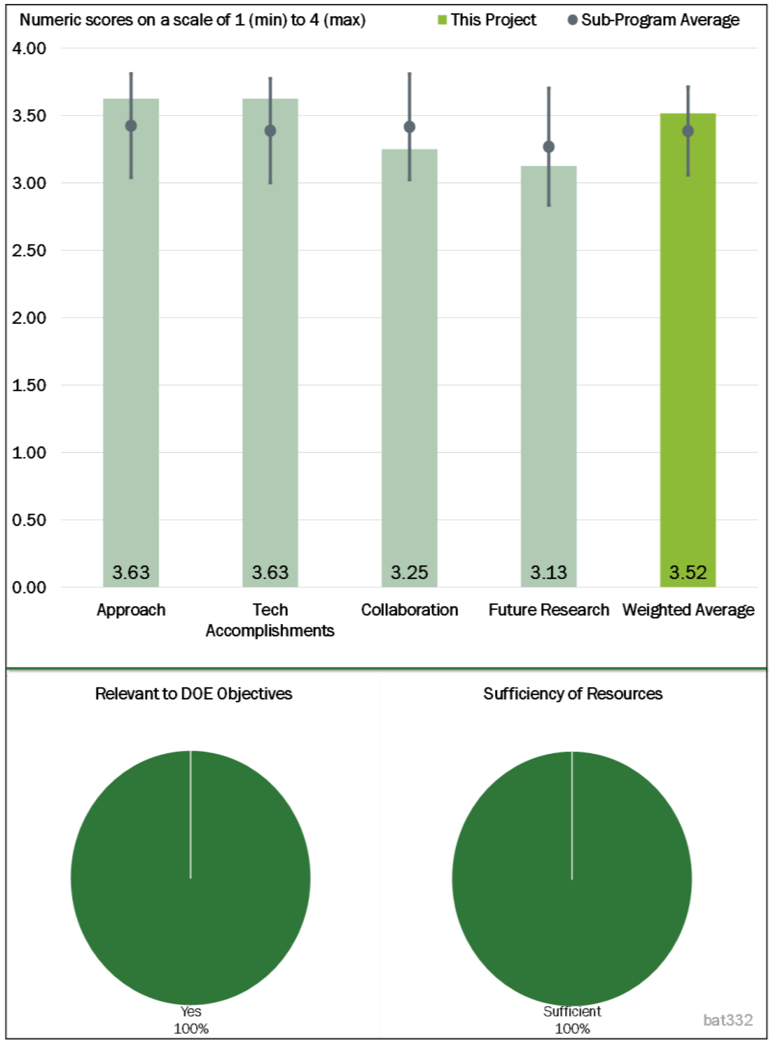

Figure 2-44 - Presentation Number: bat332 Presentation Title: High Electrode Loading Electric Vehicle Cell Principal Investigator: Mohamed Taggougui (24M Technologies)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer commented a revolutionary improvement in how to make electrodes and cells.

Reviewer 2:

The reviewer observed a very good understanding of the practical limitations on electrode design and production at high volume. The reviewer had some concern about market adoption of single side coated electrodes into high-volume cell assembly and ability to roll-to-roll (R2R) produce and process the electrodes. The reviewer said that pot life and fill/formation protocols are acceptable for transfer to industry.

Reviewer 3:

The reviewer pointed out that regarding ruggedness, the project team got the European Council for Automotive R&D (EUCAR) classification of EUCAR 1, and the pressure test shows no leaking, fire, explosion, or exothermical reaction. However, other issues, such as cost and performance, are not mentioned. The reviewer recommended that the project needs to address abuse, tolerance, and reliability barriers collectively.

Reviewer 4:

The reviewer said very interesting concept with a thick electrode, and the project needs to perform extensive rate and cycling studies, and a cost evaluation of the pre-lithiation step.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said tens of thousands of cells, and commented that because the team has substantially reduced the amount of non-active material in the cells, an enormous cost advantage is possible

Reviewer 2:

The reviewer said that the team has made clear strides in cell development and testing, and the team needs to evaluate rate and elevated temperature stability.

Reviewer 3:

The reviewer said that the team has done a good job addressing issues with viscosity limits of high solid loading electrodes. The reviewer pointed out there may be an issue with vehicle adoption, but other significant low-cost energy storage markets can be pursued. The reviewer noted that abuse tolerance benefits may compensate for Wh/L Wh/$ trades for lower solid loading. The reviewer pointed out that the references to pre-lithiation and Si volume expansion are tantalizing but not substantiated.

Reviewer 4:

The reviewer pointed out that the entire program is progressing objectively. However, improvement of the energy density is needed, beyond the 64.5% of program goal; though the team completed the reduction of use of inactive material, as well the abuse tolerant battery systems and the mass production.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said good collaboration and coordination with partners.

Reviewer 2:

The reviewer noted that partnerships in all parts of the world have been set up. The team has backing from a large energy company

Reviewer 3:

The reviewer said collaboration looks to be only with 24M, and that the team should work with Sandia National Laboratories on testing.

Reviewer 4:

The reviewer said neutral score, and elaborated no funded collaborators on program, but no obvious capability gaps either

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

Reviewer 1:

The reviewer said that the spending pace seems to be lagging a bit, but very good identification and prioritization of the gaps in commercialization.

Reviewer 2:

The reviewer said that future work well-coordinated with the design and system working. The next step is the coating, which is needed for one of the team's goals to eliminate barriers.

Reviewer 3:

The reviewer commented that the company wants to supply the automotive industry. There are some possible drawbacks. The reviewer pointed out that auto suppliers traditionally are not very profitable. The reviewer said that the project's power capability may not be good enough for vehicles, but they are in a great position for grid storage.

Reviewer 4:

The reviewer described proposed future research as overly broad and vague, and indicated the need to identify challenges or else this project should be deemed a success.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that the project definitely meets DOE objectives with reducing cost of EV batteries to spur vehicle electrification and domestic production, and that the project should also be relevant to the grid. The reviewer said that this is an exemplary DOE program in terms of technical risk/reward and solid understanding of scale up.

Reviewer 2:

The reviewer said that the project supports DOE objectives as it plans to increase the energy density and ruggedness of a battery, which is highly needed for EVs.

Reviewer 3:

The reviewer pointed out a big cost reduction for grid storage.

Reviewer 4:

In this reviewer's opinion, reducing copper will be a significant improvement and help drive down the cost of the cells. The reviewer recommended that future work should include economic analysis of the cell and components.

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 resources are sufficient.

Reviewer 2:

The reviewer said that resources are sufficient, considering that the team needs to increase the energy density by 35.5% to reach the program goal.

Reviewer 3:

The reviewer said that 24M is making timely progress against milestones.

Reviewer 4:

The reviewer said that resources are okay.

Presentation Number: bat344
Presentation Title: Electrolyte Reactivity and Its Implication for Solid-Electrolyte Interface (SEI) Formation
Principal Investigator: Kristin Persson (Lawrence Berkeley National Laboratory)

Presenter

Kristin Persson, Lawrence Berkeley National Laboratory

Reviewer Sample Size

A total of six reviewers evaluated this project.

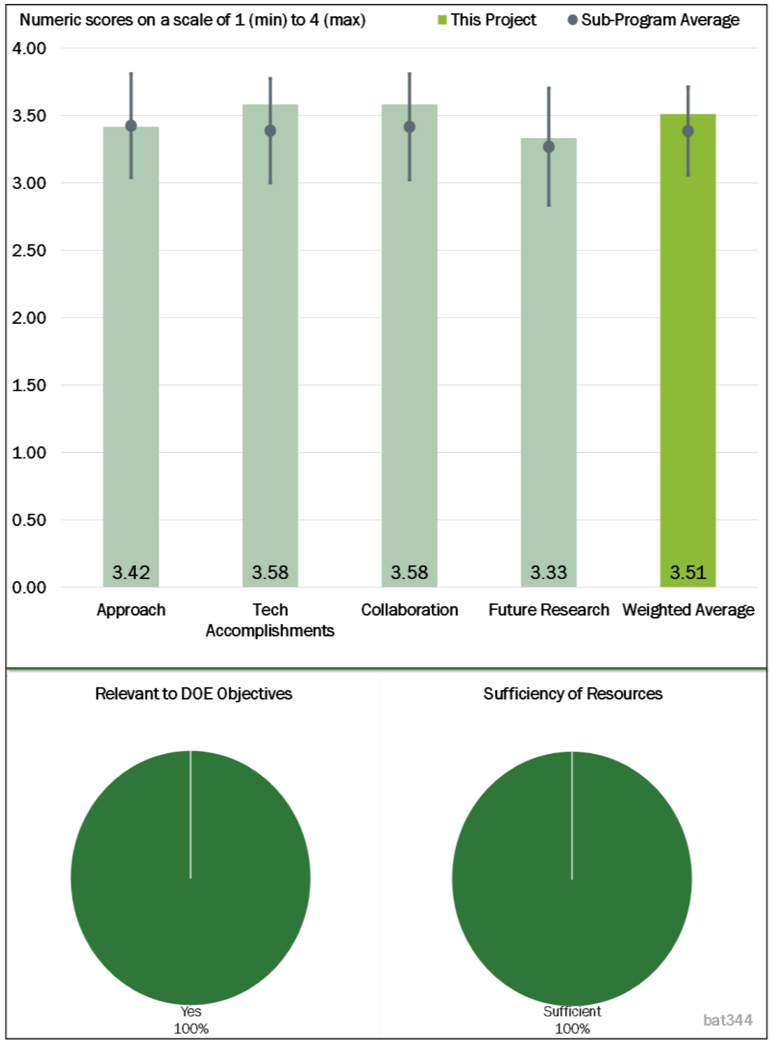

Figure 2-46 - Presentation Number: bat344 Presentation Title: Electrolyte Reactivity and Its Implication for Solid-Electrolyte Interface (SEI) Formation Principal Investigator: Kristin Persson (Lawrence Berkeley National Laboratory)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer said that this project aims at the interfacial chemistry between Si anode and electrolyte. With extensive cooperation, the project team combines the computational and experimental methods to probe the underlying science of the SEI formation as a function of electrolyte formulation, Si surface composition, and battery cycling. The reviewer said that the achievements in this project are promising to inspire and guide the mechanism study as well as material engineering for an advanced Si anode, which is significant in the development of next-generation and commercially viable Li-ion batteries. The feasibility of this project is good, the scheduling is reasonable, and considerable staged results have been achieved. The reviewer expressed optimism that the project can be well-accomplished on time.

Reviewer 2:

The reviewer commented that this is a well-thought out, well-planned team project to characterize the surface reactions that take place on Si (and related materials), and the approaches are outstanding. However, that is not the only key barrier that needs to be addressed—especially the electro-mechanical aspects of the reactions. The reviewer did not see that aspect of the work being an integral part of the studies.

Reviewer 3:

The reviewer said that the researcher addressed the strengths and weaknesses of the technical barriers clearly. The reviewer said that the project is using molecular dynamics calculations to understand the problem, and noted clearly defined research carried out a feasible way.

Reviewer 4:

The reviewer said that this project was one of the multiple projects aiming for a better understanding of interaction between electrolyte and Si-based anodes. This work provides the first step of understanding through thermodynamic calculations and validations.

Reviewer 5:

The reviewer remarked very nice work; important and informative. The reviewer noted that the project is well-connected to the other DOE Si projects. The reviewer said that the project could be improved by better (and direct, instead of just relevant literature) experimental support to validate the conclusions.

Reviewer 6:

The reviewer said that the first-principles and simulation-based work is well-designed and provides excellent support of, direction for, and validation of much of the more experimental activity of the other partners in the Silicon Electrolyte Interface Stabilization (SIESta) team.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted excellent technical progress with very impressive results has been achieved in this project. It is gratifying to see how much can be modeled today using the latest computational techniques and resources and more importantly how well these data align with experimental values. The reviewer said that calculating the percentages of solvent-separated or contact ion-pairs as a function of additives, their impact on reduction potential at different surfaces, etc., provide important theoretical insights to understanding SEI characteristics of Si-based anodes.

Reviewer 2:

The reviewer said that the combination of theoretical, experimental, and simulation strengthens the progress of the overall project. The reviewer said that relevant correlations have been established against performance indicators.

Reviewer 3:

The reviewer said that the project is on-track.

Reviewer 4:

The reviewer said that it is very nice to see the fundamental studies of electrolyte species in bulk electrolyte, a Si anode, and their interface with and without additives. The project team validated simulation results with various experiments confirming the accuracy of calculations. The reviewer said that it would be nice to expand this type of research with more practical electrolyte combinations.

Reviewer 5:

The reviewer pointed out that it is claimed that higher temperature favors the formation of contact ion pairs in both bulk and at the interface. However, the related information is missing. The reviewer explained that the extent of such impact as well as the underlying mechanism is worthy of investigation because the temperature-induced performance fluctuation is very important and challenging in battery development.

As demonstrated, this reviewer indicated that Li diffusion in the native surface SiO_2 is a kinetic bottleneck for lithiation of Si anode. The reviewer asked what the possible solution is to such a kinetic barrier. Additionally, the reviewer inquired about the SEI formation reactions when the SiO_2 shell was artificially stripped (or on pure Si surface).

Reviewer 6:
The reviewer noted useful findings, in particular regarding the voltage-based stability, and the phase and voltage profile phenomena.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer observed a superb collaboration team.

Reviewer 2:
The reviewer commented that including different DOE national laboratories’ expertise and researchers from academia is very thoughtful and enables the author to perform the mission very well.

Reviewer 3:
The reviewer said that through collaboration with various national laboratories and universities, each calculation was verified with empirical data.

Reviewer 4:
The reviewer remarked that project partners participated actively and are well-coordinated.

Reviewer 5:
The reviewer commented that collaboration on the project within the national laboratory system partners appears to be and should be able to be well-coordinated. The reviewer said that collaboration with university partners appears to be well-coordinated as well. The reviewer was concerned about an absence of any partnership with an industrial electrolyte supplier and this could limit maximum relevance.

Reviewer 6:
The reviewer remarked that coordination was well-connected within DOE, but please seek experimental support to validate the conclusions.

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 pointed out that ESI is a known phenomenon and the author has identified different approaches to address this in future research proposal.

Reviewer 2:
The reviewer found that the future direction is clear and relevant.

Reviewer 3:
The reviewer said that the proposed future research is logical, including milestones and risk management.

Reviewer 4:
The proposed work exploring interfacial speciation, their characterization, impact of different electrolytes on SEI, etc. all look good. The reviewer recommended including the mechanical aspects to this work. The reviewer asked if the swelling characteristics can be estimated as a function of electrolytes, and alloy compositions.

Reviewer 5:
The reviewer commented that the plan to focus on early SEI components and subsequent disposition is excellent. The reviewer suggested that additional focus areas for further consideration could include related impact of cathode and/or binder decomposition products in electrolyte.

Reviewer 6:
The reviewer said that the team has a solid plan for the next step. However, it would be nicer to look at broader research results with more practical electrolyte compositions or SiO_x, which is more favorable to the Li-ion battery industries.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer agreed yes, the project supports DOE's overall objectives in advancing the path towards energy density increase via Si-anode implementation.

Reviewer 2:
The reviewer said that cost, performance, and safety are the DOE objectives with respect to batteries and the author clearly identified these at the onset of the research.

Reviewer 3:
The reviewer commented that the Si-based anode is the choice for delivery of an advanced Li-ion battery with higher energy density and low cost, which has a great potential to meet DOE's goals for EVs. The fundamental studies through this project can give a better understanding of the electrochemistry of a Si-based anode and electrolyte providing clues on how to tackle the major life issues associated with Si-based anodes.

Reviewer 4:
The reviewer said that DOE's goals to understand and improve Si negative materials are important and relevant to industry. The fundamental modeling effort is an important and necessary part of this work.

Reviewer 5:
The reviewer commented that this project supports the overall DOE objectives, the development of PHEVs and EV batteries that meet or exceed the DOE and USABC goals.

Reviewer 6:
The reviewer found that better insights into the SEI characteristics of the Si anode clearly have relevance to the overall DOE objectives of developing better battery technologies. However, as is now well-accepted, mere understanding and improving the SEI characteristics alone will not allow the Si-based anode to be developed into a practically useful anode. The swelling features need to be understood and contained and that did not receive that much focus in the overall project (not this specific project only).

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

Reviewer 1:
The reviewer found that the research team has sufficient funding, human resources, and equipment to complete the project.

Reviewer 2:
The reviewer commented that resources appear in-line with work plan.

Reviewer 3:
The reviewer said that the PI and the project team have deep knowledge on the molecular dynamics. LBNL has electrochemistry teams who can support this project within LBNL but through a well set-up collaboration with various national laboratories and universities, technical support, and direction can be provided for delivery of meaningful results.

Reviewer 4:
The reviewer said that relative to other projects, the resources seem significant, but appropriate given the scope of activity and the number of partners.

Reviewer 5:
The reviewer said that with involvement from academia and different DOE national laboratories, resources are plenty for this research.

Reviewer 6:
The reviewer referenced prior comments. The reviewer was a bit unclear whether the $3.9 million was used only for this project (which sounds very, very high) or among the consortium members.

Presentation Number: bat345
Presentation Title: Chemical Reactivity of Silicon at the Surface
Principal Investigator: Gabe Veith (Oak Ridge National Laboratory)

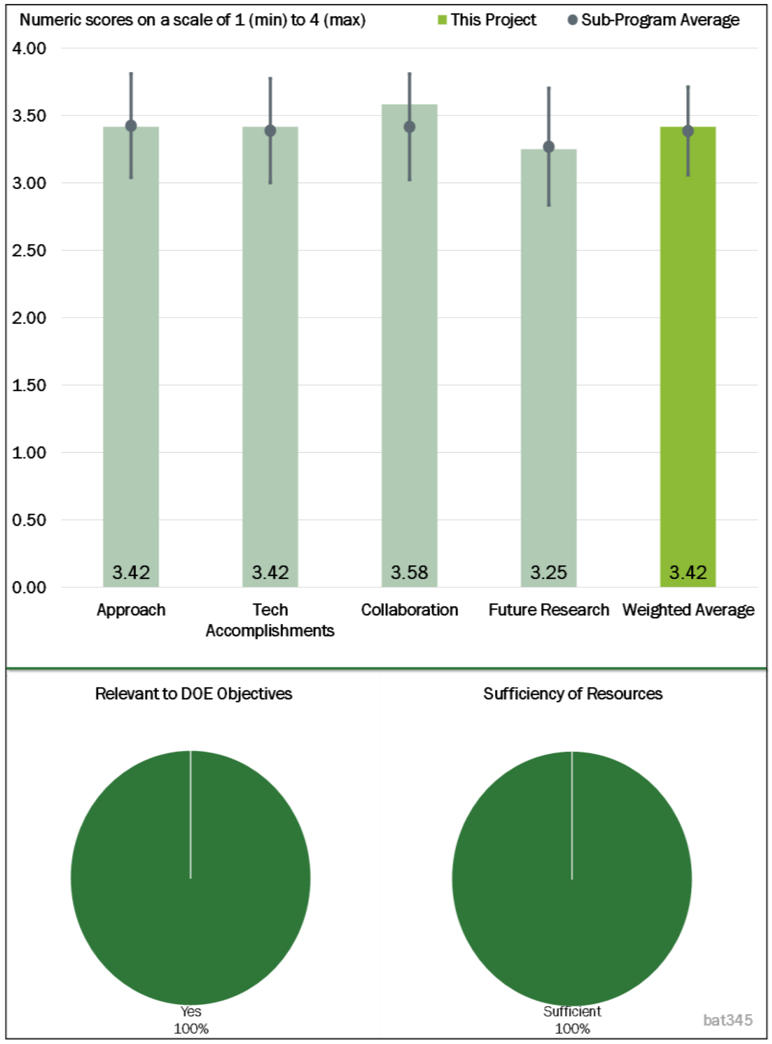

Figure 2-47 - Presentation Number: bat345 Presentation Title: Chemical Reactivity of Silicon at the Surface Principal Investigator: Gabe Veith (Oak Ridge National Laboratory)

Presenter
Gabe Veith, Oak Ridge 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 and well-planned.

Reviewer 1:
The reviewer noted a very effective approach built on extensive collaboration and standardization of materials and architectures. The reviewer commented very well-designed work progress.

Reviewer 2:
It is a very focused and well-planned approach entailing several common as well as novel techniques such as tip-enhanced Raman spectroscopy (TERS) and neutron reflectometry to characterize chemical reactions that take place on Si and analogous material surfaces as well as other electrode components when in contact with electrolytes as a function of time. However, as noted in other projects of this consortium, and in this reviewer’s opinion, including a work that would also look at the chemical reactions on the Si materials once they have undergone swelling/pulverization would also be very instructive.

Reviewer 3:
The approach seems well-planned and well-executed so far with very useful resulting findings coming from practical and feasible experimental observations.

Reviewer 4:
The reviewer said that the approach is good and the project contributes to achieve the overall goals of the SEI stabilization (SEISta) program. This project also prepares standard Si thin film samples as one of the model systems distributing among various projects. The reviewer said that the FTIR technique was heavily used in the studies. The reviewer pointed out that while it is effective with certain gases, not all gases produced during the reactions may be detected. The reviewer recommended bringing in other analytical techniques such as mass spectrometry in gaining better understanding of the gassing behavior of Si-anode materials.

Reviewer 5:

The reviewer remarked very interesting study. The time to reaction onset needs to be further investigated to understand the mechanism. The reviewer thought that the experimental setup was very well done, with built in checks for contamination/leaks.

Reviewer 6:

The reviewer remarked that the research objective is not often handled by other organizations and interesting. However, the approaches to resolve the possible issues are not clearly addressed at the beginning of the talk. The reviewer said that it was clearer through detailed review of the presentation.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said extensive studies with well-defined Si material surfaces with temporal monitoring and characterization of the products as a function of electrolytes have led to a rich set of results that provide very useful insights into the nature of the gaseous products and the associated surface chemistries.

Reviewer 2:

The reviewer said that the researcher's effort to understand the changes in material behavior is very effective to achieve the overall project success. The researcher attempted to capture as much quantitative information as possible to understand the surface characteristics.

Reviewer 3:

The reviewer found that the project has made significant progress. The reviewer wondered why the gassing studies were only limited to conditions under chemical reactions. It seems rather important to perform these studies under both chemical and electrochemical conditions. One cannot really separate chemical and electrochemical processes or gaseous versus non-gaseous products.

The reviewer recommended better characterization of the Si surface properties, especially in the dissolution studies. The nature of the surfaces oxide has large influence on the dissolution behavior. On the same front, better control of the liquid electrolyte quality is important in order to get meaningful results. The reviewer would like to understand how electrolyte quality was ensured for the studies. The reviewer would also like to see more linking between insights learned from these specific studies and how they would be used to improve performance and stability of the real-world Si-anode materials. The reviewer was not clear how all these understanding will ultimately be used to advance Si-anode materials.

Reviewer 4:

The reviewer pointed out that electrolyte reactivity with Si materials is a complex but critical to understand topic. Even though there is still a very long way to go, this project showed progress towards a better understanding.

Reviewer 5:

The reviewer said that it was very practical to try running experiments with various Si-based materials and electrolyte compositions to back up the major findings. However, according to the reviewer it would be better to include more details on possible mechanisms of the chemical reactions presented.

Reviewer 6:

The reviewer commented that although significant results were obtained with most of the areas studied and techniques applied, the gas evolution observations, while not trivial to carry out, seem in particular to have provided key and tangible findings. The reviewer found that of all of the methods applied or developed, the TERS output so far seems to be the least useful in terms of tangible advancement in understanding.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found that the project had excellent collaboration among the teams with complementary strengths and roles.

Reviewer 2:
The reviewer said that a broad-based collaboration among DOE national laboratories and academic institution researchers strengthens the analysis.

Reviewer 3:
The reviewer said that some of the key findings were obtained through various analyses techniques from collaborators. The authors nicely referred to the projects that specifically focus on the analytical techniques.

Reviewer 4:
The reviewer said that the project was well coordinated with other DOE Si projects.

Reviewer 5:
The reviewer said that collaboration on the project within the national laboratory partners appears to be and should be able to be well-coordinated. The reviewer found that collaboration with university partners appears to be well-coordinated as well. The reviewer pointed out that the absence of any partnership with industrial electrolyte supplier may be of some concern and could limit maximum relevance.

Reviewer 6:
The reviewer said that collaboration across the team is excellent. However, the reviewer noticed that there appears to be significant overlap among the individual Si projects within the SEISta program. BAT345, 346, and 347 are especially closely related and perhaps better combined into one larger project so that studies are better coordinated to minimize duplication.

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

Reviewer 1:
The reviewer said that the proposed future research clearly identifies the technology gap and risks in the project. The researcher attempted several known risk mitigation strategies.

Reviewer 2:
The reviewer said that the future direction is clear and relevant.

Reviewer 3:
The reviewer noted that in initial phases, investigation of chemical activity of Si anode surface was a focus. Prior to varying experimental design parameter change for the next steps, the reviewer recommended scrutinizing mechanisms of gas and surface film formations for better understanding of surface chemistries and plan for the future research.

Reviewer 4:
The reviewer said that the proposed future work entailing the effect of material composition and surface looks good. However, that work more than likely will not be enough to design a Si anode that will be functionally robust enough for long-term cycling. The reviewer recommended that this work needs to be complemented by studies that addresses the large swelling of the Si anode.

Reviewer 5:

The reviewer said that overall, the proposed future work is logical. Considering gassing impacts the entire cell and cross talk is known to exist, the reviewer recommended that full cell studies are performed in the future. The reviewer recommended that in order to stay relevant to the real working Si anode materials, other model systems should be created and examined. One recommendation is to build model systems based on the knowledge currently existing in the literature and in the industry, particularly in terms of surface properties. The reviewer pointed out that the industry has had great success in developing Si anode materials over the years and there is a vast amount of knowledge on what works well and what does not. In that sense, bringing in an industry partner would greatly strengthen the effort. In addition to the native Si surface, SEI on Si is known to be affected by electrolytes and additives used. The reviewer suggested incorporating more electrolyte work to speed up the learnings.

Reviewer 6:

The reviewer said that the proposed future research seems excellent and should result in even greater relevance and findings for the overall project. The intent and timing to introduce greater complexity (binder, carbon black, etc.) of factors into observations is excellent. The reviewer said that including trace quantities of cathode decomposition products into the electrolyte could be a further additional step towards results of interest.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that understanding surface reactivity is a key requirement for developing a stable Si anode and hence this project does meet the DOE overall objectives of developing a high-energy battery to facilitate EV adoption.

Reviewer 2:

The reviewer commented that a newer anode material to enhance the current battery technology is one of the key DOE objectives and this research perfectly fits the objectives.

Reviewer 3:

The reviewer remarked that the outcome of this research can improve understanding of initial stages of SEI formation on Si anode providing direction for experimental design change and material selections for improvement of life of advanced battery technologies.

Reviewer 4:

The reviewer said that improving the performance of Si anode material is critical in achieving the high energy density needed in next-generation Li batteries. The project supports the overall DOE objectives and it is very relevant.

Reviewer 5:

The reviewer agreed that yes, the project supports overall DOE objectives in advancing the path towards energy density increase via Si anode implementation.

Reviewer 6:

The reviewer cautioned please be careful to maintain relevance especially given the dwell time to reaction. The reviewer said that industrial users will not wait hours before forming the cell.

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

Reviewer 1:
The reviewer said that the involvement of different DOE national laboratory researchers and well-established academic institution resources are very helpful and sufficient to achieve the milestones and deliverables on time.

Reviewer 2:
The reviewer remarked that resources are in-line with the work plan.

Reviewer 3:
The reviewer said that a breakdown of funds to individual national laboratories would have been helpful in answering this question. But judging from the work scope, it appeared to the reviewer that the funds are sufficient.

Reviewer 4:
The reviewer said that the project teamed up with other research organizations for extensive surface analyses using various techniques. The reviewer said that an additional team for modeling possible mechanisms of film and gas formations would be beneficial.

Reviewer 5:
The reviewer was unclear how much funding this project receives so it was difficult for the reviewer to judge whether or not enough resources are available. However, the overall SEISta program has sufficient resources.

Reviewer 6:
The reviewer said that relative to other projects, the resources seem significant, but appropriate given the scope of activity and the number of partners.

Presentation Number: bat346
Presentation Title: Spectroelectrochemistry of Silicon Model Electrodes
Principal Investigator: Robert Kostecki (Lawrence Berkeley National Laboratory)

Presenter

Robert Kostecki, Lawrence Berkeley 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 and well-planned.

Reviewer 1:

The reviewer remarked that the researcher's analysis is sharply focused on barriers and underlying cause. The well-designed project effectively addresses the technical barriers.

Reviewer 2:

The reviewer said that the project has a sharp focus to characterize key components of the SEI layer that forms on Si materials utilizing an array of spectroscopic tools. The approach is well-planned and comprehensive.

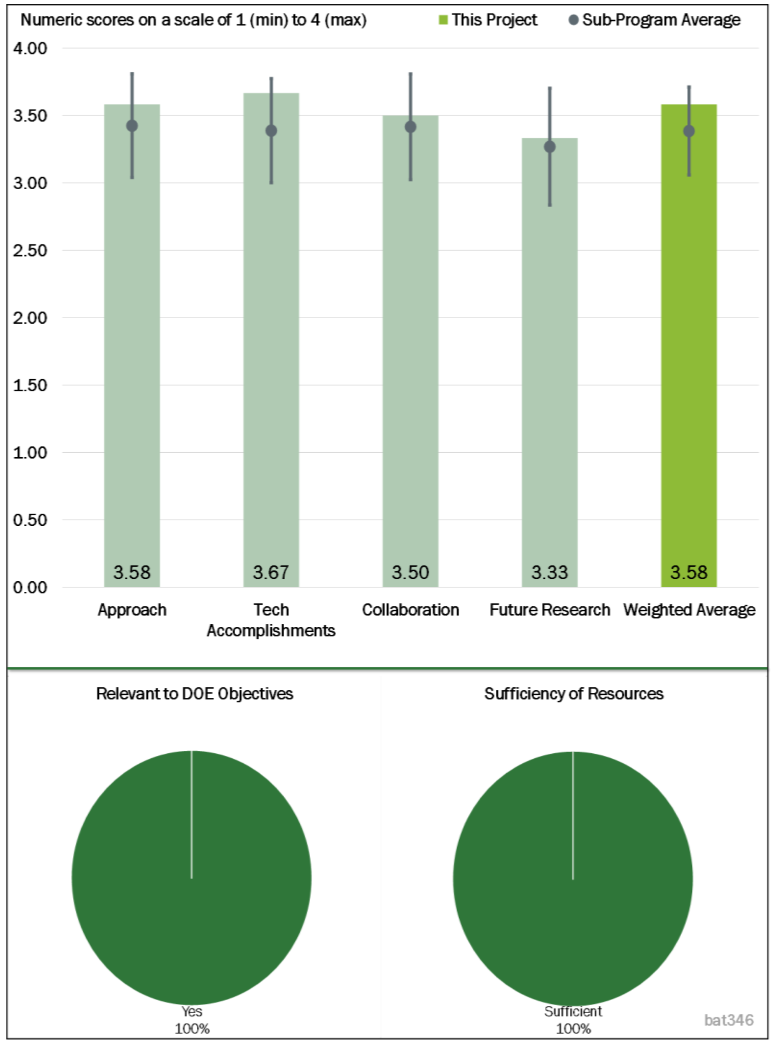

Figure 2-48 - Presentation Number: bat346 Presentation Title: Spectroelectrochemistry of Silicon Model Electrodes Principal Investigator: Robert Kostecki (Lawrence Berkeley National Laboratory)

Reviewer 3:

The reviewer remarked that the project nicely balances its own work and information from the literature for possible explanations of SEI layer appearance/disappearance during cycling, and mechanisms of each constituent of the SEI layer on a Si anode.

Reviewer 4:

The reviewer observed a unique and innovative approach. The reviewer said that results are very informative and critical to understand.

Reviewer 5:

The reviewer said that the project work is well-focused with the application of select analytical techniques and dynamic behavior of SEI on model materials with cycling.

Reviewer 6:

The reviewer detailed that this project involves the development a novel Li-ion negative electrode based on Si as the active material. The project so far includes the characterization of SEISta model research samples by

XPS, secondary ion mass spectroscopy (SIMS), IR, and Raman before and after contact with electrolyte, before cycling, and characterizes the nature of the electrolyte decomposition products in SEI. The team is also investigating the growth rate of SEI layer at fixed potential during cycling. The reviewer suggested that the authors also try to correlate SEI layer growth rate to the crack formation and propagation during cycling. The reviewer said that this could be obtained by taking various SEM/TEM images at different cycles.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that the project has made significant progress towards its technical goals with high-quality results. Using a variety of tools such as XPS, SIMS, and Raman, the team was able to identify and monitor key SEI components such as LiEDC as a function of lithiation and de-lithiation. The reviewer found that data that unambiguously showed the appearance and reappearance of species such as LiEDC are quite insightful and instructive.

Reviewer 2:

The reviewer said that this work is going a long way toward further understanding (if not yet mitigating) the SEI instability on Si surfaces.

Reviewer 3:

The reviewer said that the researcher performed extensive analysis to understand the lithiation/de-lithiation between different cycles both qualitatively and quantitatively. The reviewer remarked that the researcher made several key observations to establish the relationship between SEI thickness and composition in relation to SOC.

Reviewer 4:

The reviewer commented that the research team showed evidence of SEI layer composition on Li-silicate during charge and discharge using spectro-electrochemistry analytical techniques and offered the insights into dynamic behavior of the pseudo passivation layer during cycling. An outcome of this research will be a good reference for tackling the issue associated with an unstable passivation layer on a Si-anode.

Reviewer 5:

The reviewer said that findings via ATR FTIR in understanding the dynamic behavior of SEI on model materials at varying degrees of lithiation seems of particular value in better understanding the nature of the mechanisms involved as well as in advancing the understanding of the scope of the Si SEI stability issue.

Reviewer 6:

The commented that the FTIR results are presented for the first and second lithiation/de-lithiation. The reviewer asked how the author can make sure that LiEDC re-appears for the upcoming cycles. Secondly, the reviewer asked how the Si particle size affects the SEI layer growth rate. This is because Si lithiation and de-lithiation behavior is highly depended on the particle size.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted great collaboration with ORNL and NREL for the sample electrode and the unique three-electrode cell design for the ex situ FTIR analysis.

Reviewer 2:

The reviewer noted a very well-coordinated collaboration among different DOE national laboratories and academic researchers to establish common ground for the research

Reviewer 3:

The reviewer said that the partners participated and are coordinated.

Reviewer 4:

The reviewer commented that the project is well-connected to other DOE Si projects.

Reviewer 5:

The reviewer said that the project had excellent collaboration across the various teams. The reviewer said that a team member is absent here that addresses the mechanical aspects of overall project.

Reviewer 6:

The reviewer noted collaboration on the project within the national laboratory system partners appears to be and should be able to be well-coordinated. Collaboration with university partners appears to be well-coordinated as well. The reviewer noted that the absence of any partnership with an industrial electrolyte supplier may be of some concern and could limit maximum relevance.

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 a well-thought out plan for future research to address challenges and barriers. The reviewer said that researchers identified the key questions to be addressed.

Reviewer 2:

The reviewer observed a solid work plan for the next step for characterizing various high-energy anode material candidates using the similar analytical techniques. The additional work will provide more insight into interfacial properties of the Si-anode using a new in situ FTIR and XAS measurements.

Reviewer 3:

The reviewer said that the proposed future research is logical and includes milestones and risk management.

Reviewer 4:

The reviewer said that the future direction is clear. The reviewer said the project could be further improved by linking the results to electrochemistry (dQ/dV, CE, and performance). In addition, it would be interesting to verify methods by experimenting with controls (such as Gr) that have a known, stable SEI.

Reviewer 5:

The reviewer commented that the intent for investigating modified versions of model electrode materials is excellent. The reviewer was unsure of the relative value of further development of a near-IR approach compared to already clear and valuable findings from ATR FTIR.

Reviewer 6:

The reviewer said that the proposed future research aims to further characterize the SEI components, take inventory of Li, and develop additional analytical tools to characterize interfacial phenomena as a function of cycling will address the project goals. The reviewer, however, did not see much value to digress into alternative anode work entailing tin, germanium, or antimony.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that understanding the SEI stability on Si surfaces is a critical first step to improvement. This work is focused and relevant.

Reviewer 2:
The reviewer said that identifying and characterizing key components of the SEI that forms on the Si, especially during charging and discharging, is an essential requirement to develop a stable Si anode that is in full agreement with DOE overall objectives of higher density batteries.

Reviewer 3:
The reviewer said that overall DOE objectives are met.

Reviewer 4:
The reviewer pointed out that this project involves fundamental research to tackle the barriers associated with development of an advanced Li-ion battery using a high specific energy anode offering a great potential for more efficient packaging, longer driving range, and low cost of electrified vehicles.

Reviewer 5:
The reviewer said that this project supports the overall DOE objectives, specifically the development of PHEV and EV batteries that meet or exceed DOE and USABC goals.

Reviewer 6:
The reviewer agreed yes, the project supports overall DOE objectives in advancing the path towards an energy density increase via Si anode implementation.

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

Reviewer 1:
As commented on other projects, the reviewer believed that the funding level is sufficient, although a breakdown for the individual national laboratories was not given.

Reviewer 2:
The reviewer said that the research team has sufficient funding, human resources, and equipment to complete the project.

Reviewer 3:
The reviewer said that resources are in-line with work plan.

Reviewer 4:
The reviewer said that sufficient resources have been allocated for this research. The reviewer recommended that involvement of an industry partner will augment this research from a commercial perspective.

Reviewer 5:
The reviewer remarked that the project team works efficiently based on deep knowledge on formation mechanisms of various key species of SEI layer and experience in analytical techniques. The reviewer said that collaboration with material experts extends the project team’s research capabilities with which the project goal can be met as planned.

Reviewer 6:
The reviewer said that relative to other projects, the resources seem significant, but appropriate given the scope of activity and the number of partners.

Presentation Number: bat347
Presentation Title: Surface Analysis of the Silicon Solid-Electrolyte Interface (SEI)
Principal Investigator: Chunmei Ban (National Renewable Energy Laboratory)

Presenter

Chunmei Ban, National Renewable Energy Laboratory

Reviewer Sample Size

A total of six reviewers evaluated this project.

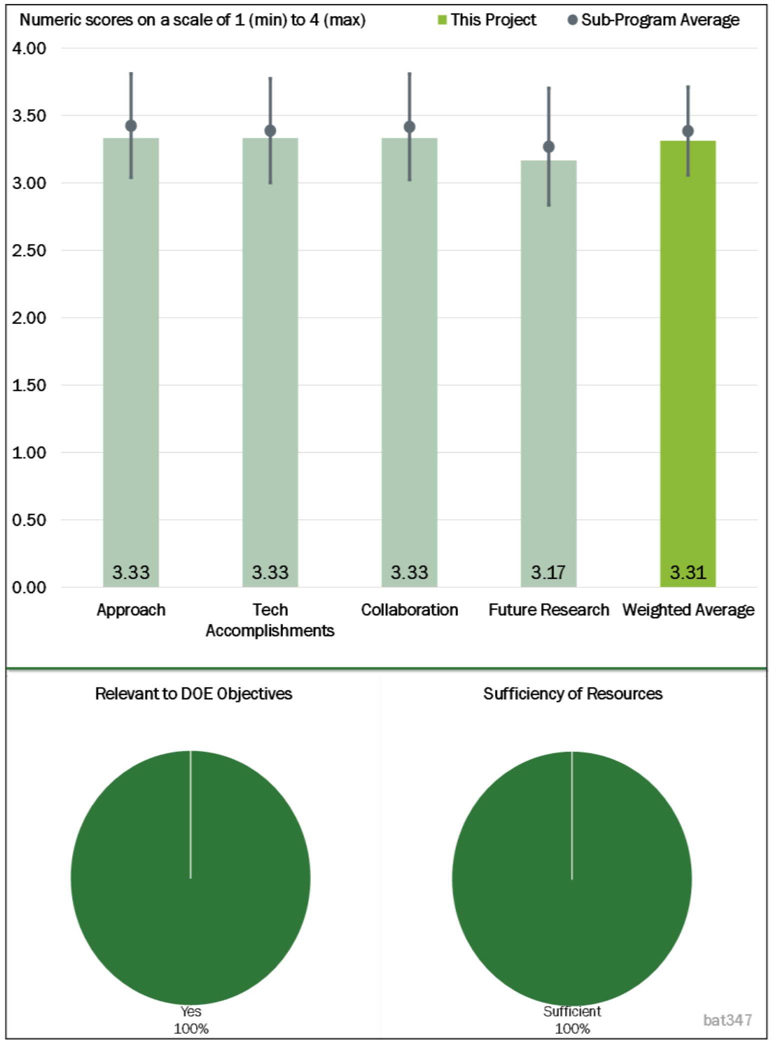

Figure 2-49 - Presentation Number: bat347 Presentation Title: Surface Analysis of the Silicon Solid-Electrolyte Interface (SEI) Principal Investigator: Chunmei Ban (National Renewable Energy Laboratory)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer said that this project has a good focus on facets of the overall Si interface issue such as thickness, conductivity, and nanostructure of the SEI that complements work carried out by other consortium members. The approach is well-thought out and well-executed.

Reviewer 2:

The reviewer commented that the researcher attempted to address certain barriers in this research. The reviewer found that overall, it is well defined.

Reviewer 3:

The reviewer noted a unique and innovative approach to understand SEI on Si.

Reviewer 4:

The reviewer found that the project appears to be somewhat of a shotgun approach to apply or develop a variety of diagnostic methods towards better understanding of Si SEI composition, structure, and electrolyte effects, and the target is hit with a number of the diagnostic approaches.

Reviewer 5:

The reviewer said that general approaches were employed to identify initial SEI layer formation on a Si anode. However, it would be more meaningful to diagnose the change (i.e., composition, dimension, etc.) associated with aging (both electrochemical cycling and thermally). The reviewer said that it would be helpful to better understand the SEI layer on a Si anode if compared to that on the well-known Gr. The reviewer said that approaches for broader work scopes would be ideal to see the effects of other active electrode layer components on the SEI layer formation.

Reviewer 6:

The reviewer remarked that overall, the project is well planned and it nicely compliments the SEISta program. Using the same model systems across the various projects is an excellent approach to gain comprehensive understanding on fundamental phenomena and processes occurring on Si anode materials. The reviewer, however, would like to see more connection to the “real world” materials, especially those produced by some of the most successful Si anode companies. The reviewer opined out that there is a vast amount of knowledge already accumulated on Si (as to what works and what does not), both in the literature and in the industry, so starting from “ground zero” may not be the fastest route to address some of the technical barriers facing researchers today.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that this project has obtained a number of interesting results that definitely provide valuable insights into the characteristics of the Si SEI. For example, the authors used novel diagnostic tools such as TERS to probe the heterogeneity of the surface down to the nanoscale level, and measured the conductivity of the SEI layer as a function of depth. The reviewer said that these are really state-of-the-art results allowing direct correlation and more importantly direct visualization of nanoscale level particles with electrolyte/surface factors.

Reviewer 2:

The reviewer said that good progress was made with excellent spectroscopy results and quantifiable data at different cycles. The reviewer remarked overall, good progress.

Reviewer 3:

The reviewer noted interesting and informative results, and that the results highlight the extremely complex nature of SEI on Si.

Reviewer 4:

The reviewer said that while not all of the diagnostic method approaches utilized may be of equal value, the scanning spread resistance microscopy (SSRM) method and results seem to indicate a particularly valuable and novel approach towards better understanding of the SEI and the impact of electrolyte composition on SEI resistance and SEI structure.

Reviewer 5:

The reviewer pointed out that this is a challenging topic and the project has made good progress on understating SEI on Si materials. Using SSRM measurements is interesting and potentially useful in understanding the electric properties of the SEI. The reviewer suggested that the PI should consider the porous nature of SEI and how that plays a role in the measurements. It is also not clear what is the depth resolution of the technique.

The reviewer would like to see more linking between insights learned from these specific studies and how they would be used to improve performance and stability of Si anode materials. The reviewer said it is not clear how all these understandings from various studies will ultimately be used to advance Si anode materials as we know today.

Reviewer 6:

The reviewer said that it is very nice to see extensive electrochemical analyses for characterization of SEI layer on a Si anode, but it would be very helpful to see similar analytical results with more electrolyte combinations and electrode components.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said that the project had excellent collaboration across the teams that possess complementary strengths.

Reviewer 2:
The reviewer noted the project established good collaboration to achieve the project goal.

Reviewer 3:
The reviewer said that the project is well coordinated with other Si DOE projects. The reviewer encouraged the team to continue collaborating closely to avoid duplicating effort.

Reviewer 4:
The reviewer pointed out that the project teamed up with the strong research collaborators. However, it would be very beneficial to include a large battery manufacturer to work with more practical and cost-effective chemistries.

Reviewer 5:
The reviewer said that collaboration across the team is obvious and it is excellent. The reviewer pointed out that there appears to be some overlapping among the individual projects within SEISta and it might be more productive if tasks are better differentiated and coordinated in achieving the overall goals. Further enhancement may be achieved by including outside experts who work in an industry setting.

Reviewer 6:
The reviewer remarked that collaboration on the project within the national laboratory partners appears to be and should be able to be well-coordinated. Collaboration with university partners appears to be well-coordinated as well. The reviewer said that the absence of any partnership with an industrial electrolyte supplier may be of some concern and could limit maximum relevance.

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

Reviewer 1:
The reviewer said that researchers identified the risks clearly and proposed a calculated mitigation strategy. The reviewer noted well-defined challenges and barriers with suitable risk mitigating proposals.

Reviewer 2:
The reviewer said that the work plan is relevant and clear.

Reviewer 3:
The reviewer commented that the plan to focus on the degree of stability of Si anodes and related aspects of SEI structure, composition, as well as presence of soluble compounds in the electrolyte, is sound. The reviewer pointed out that a greater focus on real-world Si anode surfaces (actual functional electrode active material particles or wires) may provide greater value if this is possible and does not detract from pursuing more fundamental findings.

Reviewer 4:
The reviewer pointed out that the team proposed an extensive list of future work that addresses the issues at hand. The reviewer noted how the work (like others in this program) is overly characterization-heavy, but there is a need to devote resources to understand the Si swelling and its mitigation to develop a practical solution.

Reviewer 5:

The reviewer said that overall, the proposed future work is logical and reasonable. The reviewer suggested that the surfaced physical and chemical properties of the current Si model system are better characterized. The reviewer cited as example what the nature is of the SiO_x on the surface. It is important that the model system bears resemblance to the working Si anode materials so that the learning is meaningful. The reviewer said that to stay relevant to the "real world" Si anode materials, other model systems may also need to be created and examined. The reviewer suggested that effort should also be introduced to transition the fundamental understanding gained from the model systems into practical cells for production.

Reviewer 6:

The reviewer observed a decent plan for future research but again it would be better to expand the work scope to include more materials for a practical electrode that may impact the analysis results.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that the project is very relevant to DOE's overall objectives by providing insights into the SEI characteristics of Si that will, hopefully, allow development of durable Si electrodes.

Reviewer 2:

The reviewer commented that a Si-based anode is the choice for delivery of advanced Li-ion batteries with higher energy density and low-cost and have a great potential to meet DOE's goals for EVs. The reviewer said that the fundamental electrochemistries in this project can better characterize a Si-based anode and the electrolyte interface providing clues on how to tackle the major life issues associated with Si-based anode.

Reviewer 3:

The reviewer found that the project supports DOE's overall goals. Improving the performance of the Si anode material is critical in achieving the high-energy density needed in next-generation Li batteries.

Reviewer 4:

The reviewer said yes, the project supports overall DOE objectives in advancing the path towards an energy density increase via Si anode implementation.

Reviewer 5:

The reviewer noted that the project further highlights the huge challenge of stabilizing Si. Obviously, there are many different mechanisms and stabilization is very difficult. The reviewer said that work needs to continue for further understanding the surface chemistry if there is any hope of utilizing Si in high fraction.

Reviewer 6:

The reviewer remarked that most of DOE's objectives are supported.

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

Reviewer 1:

The reviewer believed the resources are sufficient to achieve the milestone in a timely fashion.

Reviewer 2:

The reviewer noted plenty of resources were identified using academia and DOE national laboratories to deliver timely milestones.

Reviewer 3:

The reviewer found that resources are in-line with work plan.

Reviewer 4:

The reviewer said that without knowing the funding level for individual projects, it is difficult to answer this question, but the overall SEISta program has sufficient resources.

Reviewer 5:

The reviewer noted enough resources for fundamental research with limited materials, but for broader research, the reviewer recommended the involvement of battery industries.

Reviewer 6:

The reviewer said that relative to other projects, the resources seem significant, but appropriate given the scope of activity and the number of partners.

Presentation Number: bat348
Presentation Title: Synthesis and Stability of Lithium Silicate and Its Interaction with the Solid-Electrolyte Interface (SEI)
Principal Investigator: Chris Apblett (Sandia National Laboratories)

Presenter

Chris Apblett, Sandia National Laboratories

Reviewer Sample Size

A total of six reviewers evaluated this project.

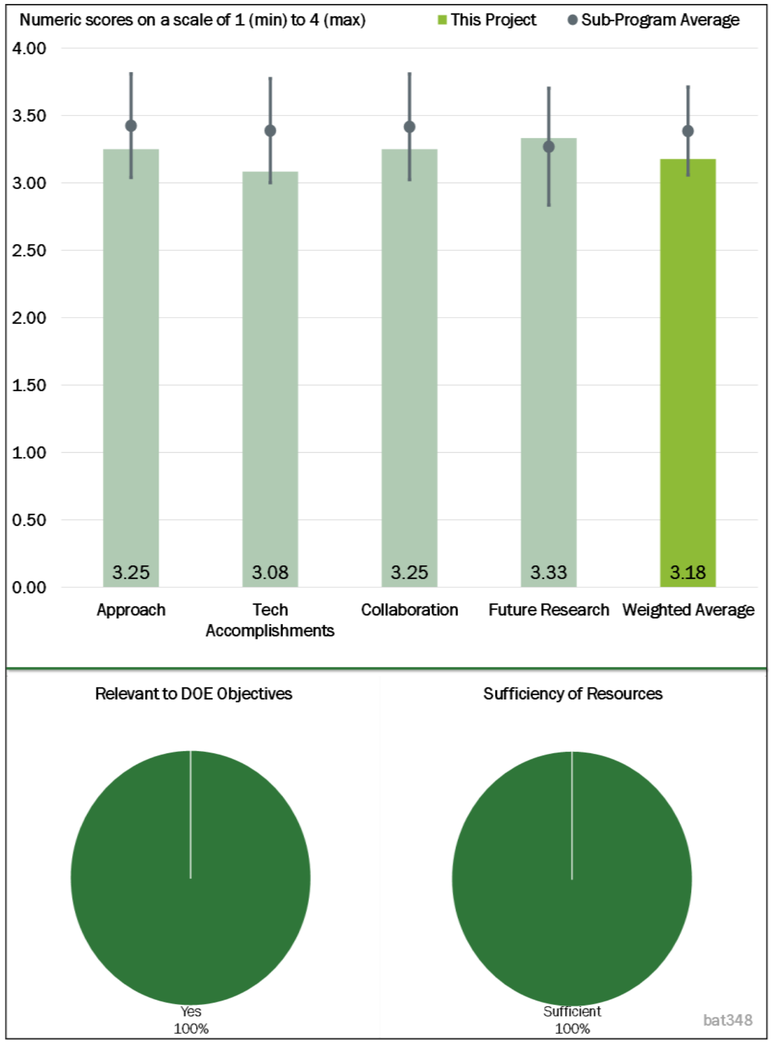

Figure 2-50 - Presentation Number: bat348 Presentation Title: Synthesis and Stability of Lithium Silicate and Its Interaction with the Solid-Electrolyte Interface (SEI) Principal Investigator: Chris Apblett (Sandia National Laboratories)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer said that this project, as a part of the overall approach to characterize Si SEI, was primarily focused on the role of the silicates, if any. This compliments the work carried out by the other team members of this consortium.

Reviewer 2:

The reviewer commented that standardized test cells for reproducibility, and using easy to assemble architectures, are good approaches to understanding the underlying technical barrier. The reviewer noted a well-developed test and analysis plan.

Reviewer 3:

The reviewer remarked that resolving the importance of silicates in Si electrodes is critical and relevant. The reviewer said that this work is unique and focused.

Reviewer 4:

The reviewer noted a well-structured approach for characterizing Li silicate on a Si anode using chemical, mechanical, and electrochemical analyses.

Reviewer 5:

The reviewer found that this work seems to be generally focused on exploring silicate phenomena, which may not have been widely or conclusively observed or understood to date. So far, while it does not seem clear what the practical outcome of this will be, the reviewer acknowledged that the project is only at a midpoint. However, involved characterization of sample materials used by the rest of the SEISta team is worthy in itself in supporting the best understanding of the entire SIESta team. The reviewer noted that elucidating the electrolyte decomposition products in the presence of uncycled electrodes must surely be of value to advancing specific understanding.

Reviewer 6:

The reviewer commented that the approach of studying model silicates to understand SEI is generally good and it complements the studies performed in the SEISta program. However, the reviewer was unclear how particular silicate model compounds (particularly chemical composition, structural properties, etc.) in this project were chosen. The reviewer wondered how relevant the results are without knowing these compounds even exist in the Si anode system.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that a thorough analysis of spectroscopic images and quantifiable data support the progress made toward the overall project. The reviewer said very informative and well thought out accomplishments towards the goal.

Reviewer 2:

The reviewer noted that the project has obtained a good amount of knowledge on some silicates. The project successfully used a number of techniques.

Reviewer 3:

The reviewer detailed how by using standard samples, the team carried out systematic studies to characterize the roles of the silicates in the SEI and measured their stability and reactivity in moisture and electrolytes using an array of analytical tools. While results are not fully unambiguous, they are quite useful in understanding whether the silicates play a dominant role or not. The reviewer found the mechanical response (modulus) studies during lithiation and de-lithiation especially insightful. The reviewer noted that impedance and SIMS results also shed further lights on the stability of the silicates.

Reviewer 4:

Progress to date appears to support the rest of the overall SIESta team, and furthers the general understanding of the SEI structure, layering, and physical properties.

Reviewer 5:

The reviewer commented that the work has identified many interesting questions so far. As the work progresses, the reviewer looks forward to more answers and solutions.

Reviewer 6:

The reviewer observed good initial observations on the behavior of various silicates with the presence of electrolytes. The reviewer expected more extensive investigations for a more robust explanation of changes during the tests (i.e., the sudden change in impedance).

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the results demonstrate excellent collaboration among the project participants.

Reviewer 2:

The reviewer said that collaboration with national laboratories seems to be effective, in particular, the design of the test cell for characterizing target materials.

Reviewer 3:

The reviewer remarked there is strong collaboration across the team.

Reviewer 4:

The reviewer observed reasonable collaboration between other DOE projects. The reviewer remarked that increased interaction with BAT344 for experimental verification of models, and with BAT345, which has similar work, could be more explicit.

Reviewer 5:

The reviewer said that most of the projects are well-coordinated between DOE national laboratories and academia. Involving an industry partner will add real-time complexity to the project and will help to find alternatives effectively.

Reviewer 6:

The reviewer said that collaboration on the project within the national laboratory system partners, appears to be and should be able to be well-coordinated. The reviewer noted that collaboration with university partners appears to be well-coordinated as well. The reviewer pointed out that the absence of any partnership with an industrial electrolyte supplier may be of some concern and could limit maximum relevance.

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

Reviewer 1:

The reviewer said that the proposed future research, including an emphasis on characterizing the sudden rise in impedance/compliant layer, and elucidating the kinetic parameters, appear good. The reviewer especially liked the team's use of the Milestone Chart, which gives a quick overview of the remaining tasks in this project. The reviewer suggested that other team-members use such a chart to help the reviewers better appreciate the work scope.

Reviewer 2:

The reviewer commented well thought-out, broad-based future research plans to support the challenges and barriers. The reviewer commented that the proposed future research clearly identified all the risks and remedial plans.

Reviewer 3:

The reviewer said that most of essential future works were well-planed and described, including the temperature effect on SEI formation on the Si anode, which other research groups did not indicate.

Reviewer 4:

The reviewer pointed out that temperature-based soaking experiments may be challenging to configure but should be valuable, and remarked that the intent to work with powder research efforts to verify phenomena in real powders is an excellent aspect of planned future work.

Reviewer 5:

The reviewer said that overall, the proposed future work is logical and reasonable. The reviewer suggested that more effort be put into real-time detection of silicates to answer questions such as whether they form, what they are, etc. The reviewer thought that perhaps new techniques can be developed to better detect silicates. Without better definition, this reviewer explained that it is difficult to construct silicate model systems and carry out detailed studies that would provide researchers with much needed insights.

Reviewer 6:
The reviewer said that future work is clear and relevant. The reviewer suggested that more details and developing a method to allow experimentation during electrochemical lithiation would be useful.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that as with the other projects in this consortium, this project has definite relevance to DOE's overall project to develop a high-energy density battery.

Reviewer 2:
This is another piece of a big puzzle in characterizing a Si-anode and finding the root causes of its aging mechanisms to deliver a robust high-energy density Li-ion battery technology. The reviewer said that like other projects, it would be great if other electrode components are included in the research for their effect on the presence of SEI layer on Si anode.

Reviewer 3:
The reviewer said that some of the projects list the common DOE objectives of cost, performance, and safety risks. The reviewer said that safety risk is not well addressed in this project, but performance objectives are well met.

Reviewer 4:
The reviewer said that understanding the role of silicates on Si SEI is very relevant and necessary.

Reviewer 5:
The reviewer found that the project supports the overall DOE objectives. Improving the performance of Si anode material is critical in achieving the high energy density needed in the next generation Li batteries.

Reviewer 6:
The reviewer agreed yes, the project supports overall DOE objectives in advancing the path towards energy density increase via Si anode implementation.

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

Reviewer 1:
The reviewer believed the funding is sufficient.

Reviewer 2:
The reviewer noted good collaboration to achieve timely milestones.

Reviewer 3:
The reviewer said that resources are in line with the work plan.

Reviewer 4:
It seemed to the reviewer that the resources are enough for the first year of research. The reviewer said that if the collaborative effort is extended with a material manufacturer (who may provide more commercial baseline material) and/or cell manufacturer (who can provide with more practical electrode), it would be very promising project.

Reviewer 5:
The reviewer said that the level of funding for this project was unclear, but the overall SEISta program has sufficient resources.

Reviewer 6:

The reviewer commented that relative to other projects, the resources seem significant, but seem more than sufficient given the scope of activity and the number of partners.

Presentation Number: bat349
Presentation Title: Research Facilities Support
Principal Investigator: Kyle Fenton (Sandia National Laboratories)

Presenter

Kyle Fenton, Sandia National Laboratories

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 and well-planned.

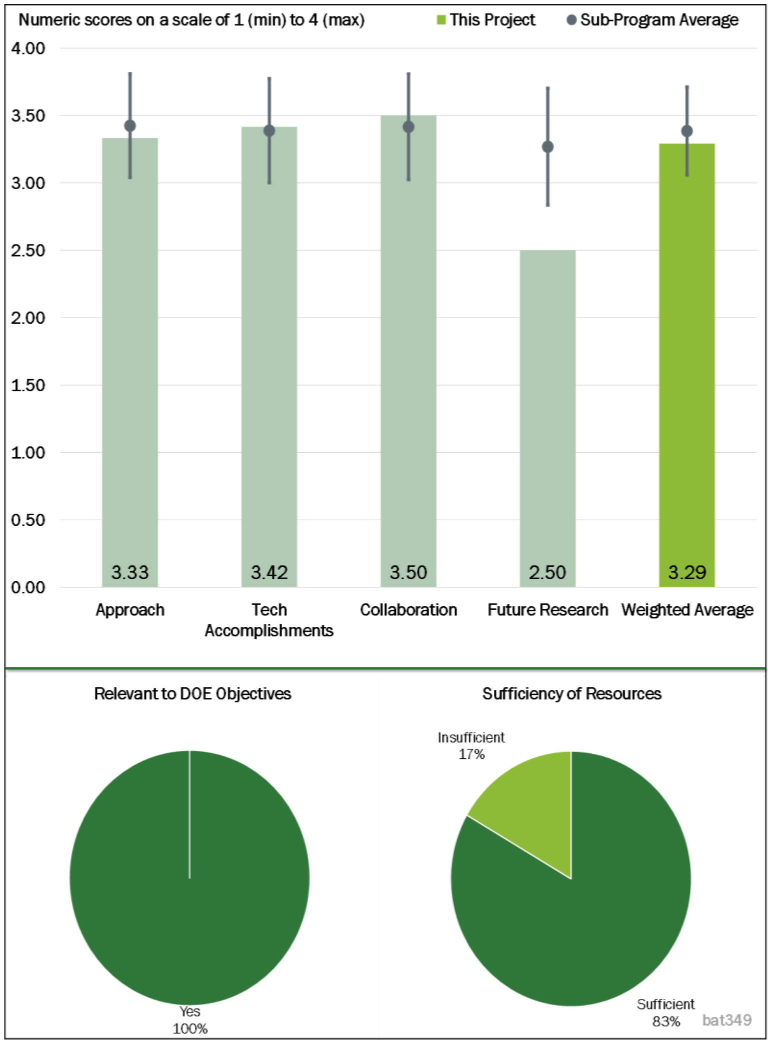

Figure 2-51 - Presentation Number: bat349 Presentation Title: Research Facilities Support Principal Investigator: Kyle Fenton (Sandia National Laboratories)

Reviewer 1:

This project has as its core focus developing and processing a Si anode that will be a viable candidate as a durable anode for high-energy Li-ion batteries. It is a multi-lab effort combining complementary strengths of the various national laboratories. The tasks are well-thought out and comprehensive except for the fact that there is too much emphasis on characterization.

Reviewer 2:

The reviewer observed clearly identified roles and responsibilities of research facilities' support to carry out the DOE technical barriers associated with battery development and overall DOE objectives. Further, this reviewer remarked that capability and feasibility are addressed very well.

Reviewer 3:

The reviewer said that the improved facilities are having a positive impact on all of the DOE Si work.

Reviewer 4:

The reviewer commented that the project takes in a wide swath of responsibility for support of Si activity in general and seems well-designed considering the breadth of activities and facilities.

Reviewer 5:

The reviewer said that the main approach of ANL's CAMP facility was informed by the change in direction of electrode design with a higher amount of Si content and a lower level of lithiation. However, the reviewer found that the target loading level (mAh/cm^2) of the electrodes in this project is not practical and even lower than state of-the-art. The reviewer suggested that a target for the loading level should be newly set up and clearly indicated for better practicality.

Reviewer 6:

The reviewer found that the approach is excellent. This is a great effort in utilizing DOE's existing large facilities and also providing an anchor for the multi-institutional projects within the Si program. The reviewer commented that the changes in direction, going from low amounts of Si and a high level of lithiation to high amounts of Si and low levels of lithiation, is a good choice. The reviewer pointed out that industry is active in pushing higher Si and it is important that a large Si program such as this one is involved in the same space. The reviewer would like to see a better connection to industrial Si anode materials. Ideally, selection of industrial material should be performance- or metrics-based rather than availability-based (as the case for the current arrangement). The reviewer understands that sometimes it is limited by availability, but because there are a number of companies producing a high-performing Si anode at this point, it seems important to stay relevant.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that the facility is excellent and still improving.

Reviewer 2:

The reviewer observed a very good analysis to identify the impurities in the Si materials. The reviewer said that it will be beneficial to highlight what performance is specifically expected instead of broad-based expectation.

Reviewer 3:

The reviewer pointed out that the data obtained on the processing of Si materials at the pilot scale, an important aspect of the work carried out in this project, showed the sensitivity to moisture/air, which is very useful. Researchers should note here, though, that it is unclear how much of these lessons learned can be transferred to Si materials that eventually become suitable for use as a durable anode. The reviewer commented that data from safety tests are very instructive and quite valuable (the reviewer did not see the capacity of the cells). Many researchers are not very aware of such challenges from the open literature.

Reviewer 4:

The reviewer said that this program has a range of milestones and broad work scopes. The reviewer found that overall, the team reported decent progress through technical facility support covering a range of milestones related to integrated activities.

Reviewer 5:

The reviewer said that significant progress has been made on understanding how processing leads to different interface terminations. The knowledge is very important in enabling high-quality Si anode materials. The reviewer observed a range of thermal behaviors in the studies. The reviewer would recommend that the group better characterize Si surface properties so that better correlation can be established. The reviewer would also like to see more effort to transition the knowledge gained from these specific studies into practical cells for production. The reviewer suggested that bringing in an industry partner would greatly strengthen the effort.

Reviewer 6:

The reviewer commented that while creating significant challenges, the findings regarding Si-based cell abuse response in accelerating rate calorimeter testing are critical to moving forward with significant Si-containing cell chemistries in a best-educated basis for the future. Additionally, the reviewer noted that gas generation studies during slurry mixing provide important insight into one novel area of the overall picture of challenges in moving forward with significant Si-containing cell chemistries.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said that the project had excellent collaboration among the consortium members.

Reviewer 2:
The reviewer remarked that collaboration with various national laboratories is the key for the success of this project, and related projects have already demonstrated the strong collaboration leading to fruitful outcomes from fundamental research on the Si-anode

Reviewer 3:
The reviewer remarked that most of the DOE national laboratories are involved in this project; this is a good coordination effort.

Reviewer 4:
The reviewer said that coordination within the Silicon Deep Dive effort is excellent.

Reviewer 5:
The reviewer found that collaboration across the project team is very strong. There is clear coordination among the institutions involved in the program.

Reviewer 6:
The reviewer commented that collaboration on the project within the national laboratory system partners appears to be and should be able to be well-coordinated.

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

Reviewer 1:
The reviewer said that proposed work, albeit very generic, is at the heart of the issue. (Interestingly none of the other project teams has specifically mentioned these topics as highlighted here). The reviewer saw as a challenge that all the other national laboratories are focusing primarily on SEI characterization and related topics. The reviewer remarked that none of the projects focused directly on how to contain swelling and make the cells durable. The reviewer said that needs to be the core effort going forward now that the characterization studies have made tremendous progress.

Reviewer 2:
The reviewer said that the future direction on synthesis is clear, but more details on other work would be appreciated.

Reviewer 3:
The reviewer said that the future research plan is not mentioned in this project.

Reviewer 4:
The reviewer said that only remaining challenges and barriers are available, and no information on proposed future research was provided in detail.

Reviewer 5:
The reviewer said that no future work was presented, and the reviewer was not sure this project is continuing.

Reviewer 6:
The reviewer said that although proposed future work does not appear to be specifically described in most areas, an assumed intent for continuation of existing work and continuation of general support for the SIESta project would be good, and is assumed in the absence of any particular descriptions.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer pointed out that without excellent research facilities, progress would not be possible. This project is relevant and necessary.

Reviewer 2:
The reviewer commented that the project is highly relevant to DOE's overall objectives of safe and cost-efficient high-energy battery by addressing issues that will enable the development of a high-capacity, durable Si anode.

Reviewer 3:
The reviewer said yes, the project supports overall DOE objectives in advancing the path towards an energy density increase via Si anode implementation.

Reviewer 4:
The reviewer remarked that research facilities support is one of the key parameters for success of battery projects to tackle the issues related to advanced battery materials and cell design.

Reviewer 5:
The reviewer said that the project supports DOE's goals of improving the performance of Si anode material to achieve high energy density.

Reviewer 6:
The reviewer said that all the DOE national laboratories have a common mission to fulfil 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 said that relative to other projects and given the scope of project activity, the resources may appear to be insufficient.

Reviewer 2:
The reviewer said that resources are sufficient except for the electrode fabrication area. The reviewer recommended benchmarking with state-of-the-art cells for more practical targets in terms of electrode design and material selections.

Reviewer 3:
The reviewer said that the resources should be sufficient to complete the tasks on schedule.

Reviewer 4:
The reviewer commented that DOE national laboratories are equipped with the best resources both tangible and intangible to achieve the milestones and to address the technical barriers in a timely fashion.

Reviewer 5:
The reviewer found that resources are in-line with work plan.

Reviewer 6:

The reviewer commented that the funding level for this project was not provided but the Si program overall has sufficient resources.

Presentation Number: bat350
Presentation Title: Electrode Characterization and Analysis
Principal Investigator: Daniel Abraham (Argonne National Laboratory)

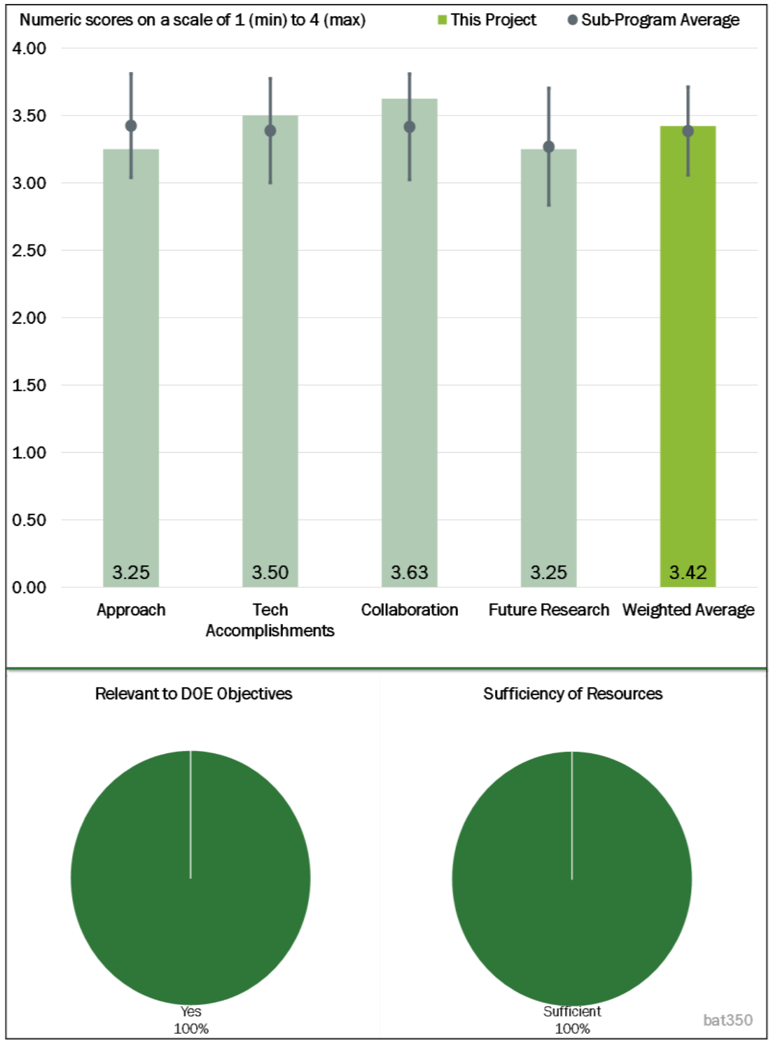

Figure 2-52 - Presentation Number: bat350 Presentation Title: Electrode Characterization and Analysis Principal Investigator: Daniel Abraham (Argonne National Laboratory)

Presenter

Steve Trask, 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 and well-planned.

Reviewer 1:

The reviewer said that advanced anode development and characterization is critical to meet NG Li-ion specific energy, energy density, cost, and life goals. Subsequently, the reviewer noted a well-defined, overall approach for the remaining Si anode solutions.

Reviewer 2:

The reviewer noted that this was a huge program and required a lot of collaborations. This project is specifically focused on electrode characterization and analysis, and the approach is well designed and will make a great contribution for this whole Si program.

Reviewer 3:

The reviewer said that overall, the approach is very comprehensive and multiple techniques are used to characterize the various issues. The reviewer said that, however, there is little discussion of the meaning and impact of the findings.

Reviewer 4:

The reviewer said that this team is spending $3.6 million per plus assistance from all of the fully funded facilities at ANL to make Si-Gr 15/73 electrodes and determine their functionality. The reviewer reported that there are two investigators listed on the title slide listed, but no one can tell whether this is the work of two investigators or five national laboratories. The reviewer noted that 20 milestones and a long list of activities are mentioned. The reviewer described the presentation as very confusing. For this group of presentations, the focus of the effort being presented does not start until the Approach slide. It is here that one finally discovers that this presentation will be an assessment of the performance of a Si/Gr electrode prepared with two different binders with regard to life, activity, and heat effects.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer believed that the work done is systematic and directly addresses project goals. Tracking the lithiation state for Si and Gr, binder and coating studies, capacity loss, and gassing investigations are all very relevant to developing efficient and effective characterizations for Si-containing materials.

Reviewer 2:
The reviewer said that of the tasks discussed in the bulk of the presentation, which the reviewer assumed were primarily performed by Trask and Abraham, good progress has been made in assessing life with regard to calendar and cycling, assessing heat release with temperature, Gr activity, and the contrasting effect of binders and solvent on performance. The reviewer thought it was interesting to see that an electrode that starts from a more uniform composition did not necessarily finish with a more uniform composition.

Reviewer 3:
The reviewer pointed out that the milestone describes the technical accomplishments for each national laboratory.

Reviewer 4:
The reviewer found that the reported work is very interesting, especially that related to relative lithiation and the effect of binders and coating. The reviewer inquired how these results depend on the specific microstructure of the C/Si composite. The reviewer said that more characterization at the microstructure level would be useful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer commented that collaboration among DOE national laboratories is excellent.

Reviewer 2:
The reviewer said that the team has diverse expertise and access to excellent facilities. There is an apparent very good coordination of efforts.

Reviewer 3:
The reviewer remarked that coordination and collaborations are very good for this big Si program.

Reviewer 4:
The reviewer said that although assuming that these are the two main investigators, there is clearly plenty of help in obtaining materials, access and assistance with several pieces of equipment. The reviewer found that despite addressing several topics, much has been learned.

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 remarked that proposed future work is focused on areas highly relevant to achieving DOE goals. These include identifying Si volume change during cycling, improving cycle life aging results, and investigating Si properties to minimize energy release and gas generation. The reviewer is also pretty excited to see the future results by using in situ Raman techniques.

Reviewer 2:
The reviewer said that optimizing electrolyte and electrode composition will help with life expectations.

Reviewer 3:
The reviewer remarked that the scope is too broad, and that more focus on specific questions may be useful. For example, the future work includes analysis of many different compositions, but researchers still do not completely understand the results at one fixed composition and how they could be dependent on electrode processing, specific chemistries, etc.

Reviewer 4:
The reviewer expressed uncertainty about what researchers will learn from operando experiments of measuring lithiation of Si as a function of Si content. The reviewer was not sure what the project team is doing with the additional inhomogeneity mapping. Hopefully, this will be combined with fabrication techniques to eliminate inhomogeneities. The reviewer expressed uncertainty about how the project team plans to minimize energy release and gas generation.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that finding a way to increase the anode specific capacity to increase energy density clearly supports DOE’s objectives.

Reviewer 2:
The reviewer remarked that understanding the mechanism of Si anodes in Li-ion batteries is really important for DOE objectives.

Reviewer 3:
The reviewer commented that the advanced anode containing Si will meet DOE energy and life targets.

Reviewer 4:
The reviewer said that this project supports DOE objectives of advancing higher capacity anode technologies.

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 resources are very reasonable.

Reviewer 2:
The reviewer remarked that resources are sufficient for this project.

Reviewer 3:
The reviewer commented that $3.6 million spending and DOE national laboratory resources should be able to support the work described in the project.

Reviewer 4:
The reviewer remarked that there is a bunch of money and physical resources being applied to develop an electrode with some Si in it. This appears to be a decent effort, but there is no clue as to how many PI’s work is being put forth in this particular presentation and what fraction of the time of the funded facilities is being occupied by this project. The reviewer said that if there was a deadline to make some defined progress, one might be able to assess how well resources are being distributed.

Presentation Number: bat351
Presentation Title: Active Particle Studies
Principal Investigator: Baris Key (Argonne National Laboratory)

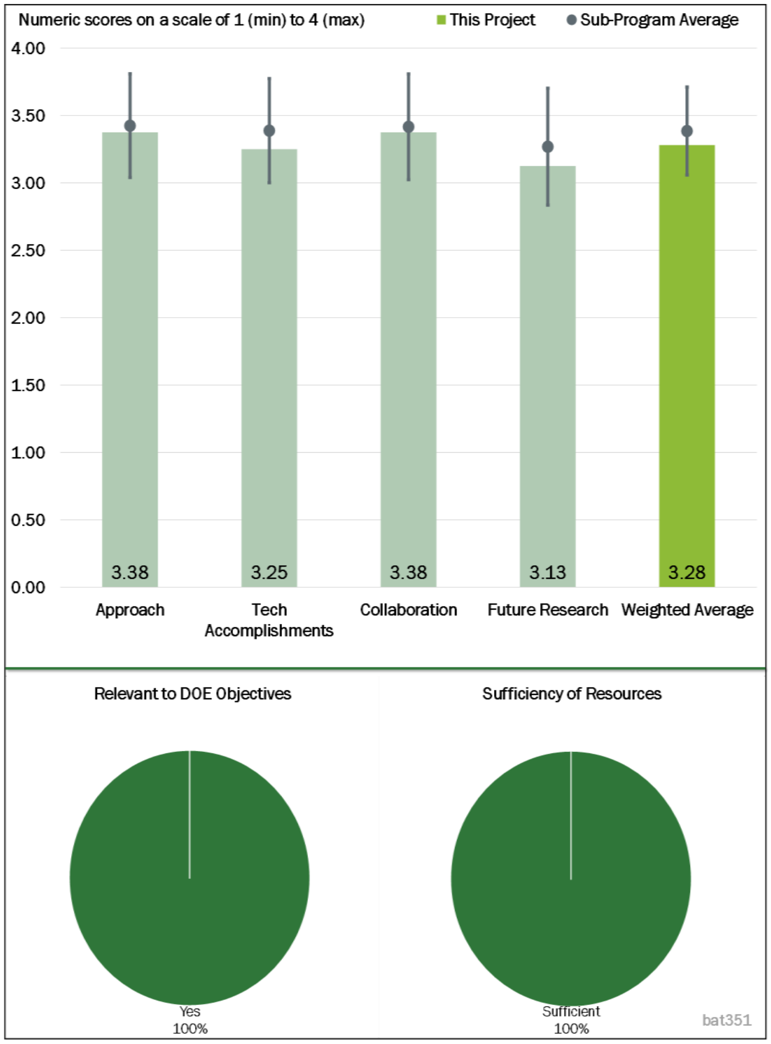

Figure 2-53 - Presentation Number: bat351 Presentation Title: Active Particle Studies Principal Investigator: Baris Key (Argonne National Laboratory)

Presenter

Baris Key, 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 and well-planned.

Reviewer 1:

The reviewer said that the project is utilizing local structure probes (NMR, FTIR, and Raman) along with diffraction is a great approach to analyzing Si materials. Li_7Si_3 is also a good start point.

Reviewer 2:

The reviewer commented that finding the most suitable Si powder, which will provide a long life and minimum self-discharge, is a good approach.

Reviewer 3:

The reviewer said that studying the reactivity of the active particles with the electrolyte and binders is useful. The reviewer pointed out that because the chemistry of these materials is very sensitive to the environment, in the context of the overall project it would be useful to consider the presence of C.

Reviewer 4:

The reviewer said that after reading the same four boiler plate slides for five presentations, reviewers finally get to the part of the presentation that finally speaks specifically to what will be seen for the next 20 minutes. It was extremely difficult for this reviewer to read the approach and have any idea if it supports what was about to follow. As it turns out, the investigator used NMR, FTIR, and Raman to study the degree of reactivity of Si compounds in the presence of different materials.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer acknowledged that there are a lot of technical accomplishments in this project. However, the reviewer noticed the investigation of triglyme-based electrolytes in this project, which is not a good choice for continuing studies. The ether is well-known for its voltage instability in Li-ion batteries.

Reviewer 2:

The reviewer remarked that studying the reactivity of the active materials (specifically Si alloys) is definitely useful, and the study is comprehensive. The reviewer pointed out that because many of these analyses have been previously done in several laboratories, it would be useful to have a comparison.

Reviewer 3:

The reviewer noted that the project utilized NMR to detect reaction of different Si compounds at different lithiations with different environments. This helped in understanding reactivity in air, against different binders, and with different components of the electrolyte. The reviewer said that the researchers need to figure out the inconsistencies between this work and results found in electrochemical cells.

Reviewer 4:

The reviewer said that the tools to study the reactivity are well applied. However, quantification to meet the 1,000 cycle and less than 1%/month self-discharge is very important to find optimized raw materials.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked overall, this is a part of big program, which has really great collaboration.

Reviewer 2:

The reviewer said that collaboration among DOE national laboratories is working well.

Reviewer 3:

The reviewer said that collaboration among the national laboratories is very good.

Reviewer 4:

The reviewer commented that the investigator effectively collaborated with a number of researchers, including those able to make cells with different active and inactive components and test and cycle cells. However, a discussion between the research results found here versus other aspects of this project appears to be lacking.

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

Reviewer 1:

The reviewer suggested that if this project is also considering the C/Si electrodes, then the contribution of C to the reactivity and stability should be studied. The reviewer concluded that proposed future research is overall very good.

Reviewer 2:

The reviewer said that the researcher intends to continue to investigate the reactivity of different systems and start to look at products from the reactivity of different electrolytes. The reviewer pointed out that the project team hopes to use this in the development of better electrolytes.

Reviewer 3:
The reviewer found that long-term future research seems reasonable, and the reviewer prefers limited studies for triglyme-based electrolytes.

Reviewer 4:
The reviewer said that the future studies should be aligned with the DOE cycle life and self-discharge requirements.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said great support for DOE objectives.

Reviewer 2:
The reviewer said that the results of the study will help to increase cycle life and calendar life.

Reviewer 3:
The reviewer said yes, because it focuses on higher capacity Si anodes.

Reviewer 4:
The reviewer detailed that by understanding the reactivity of Si with different components, the team may be able to develop a system that has the right level of reactivity that also leads to passivation. This is critical in developing the high capacity loading of Si as an anode material.

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

Reviewer 1:
The reviewer said that $3.6 million and DOE national laboratory resources are sufficient.

Reviewer 2:
The reviewer said that resources appear sufficient.

Reviewer 3:
The reviewer commented that the resources are sufficient.

Reviewer 4:
The reviewer found it impossible to comment here because the distribution of resources is so vague (and deliberately so).

Presentation Number: bat352
Presentation Title: Active Materials Advancements
Principal Investigator: Zhengcheng (John) Zhang (Argonne National Laboratory)

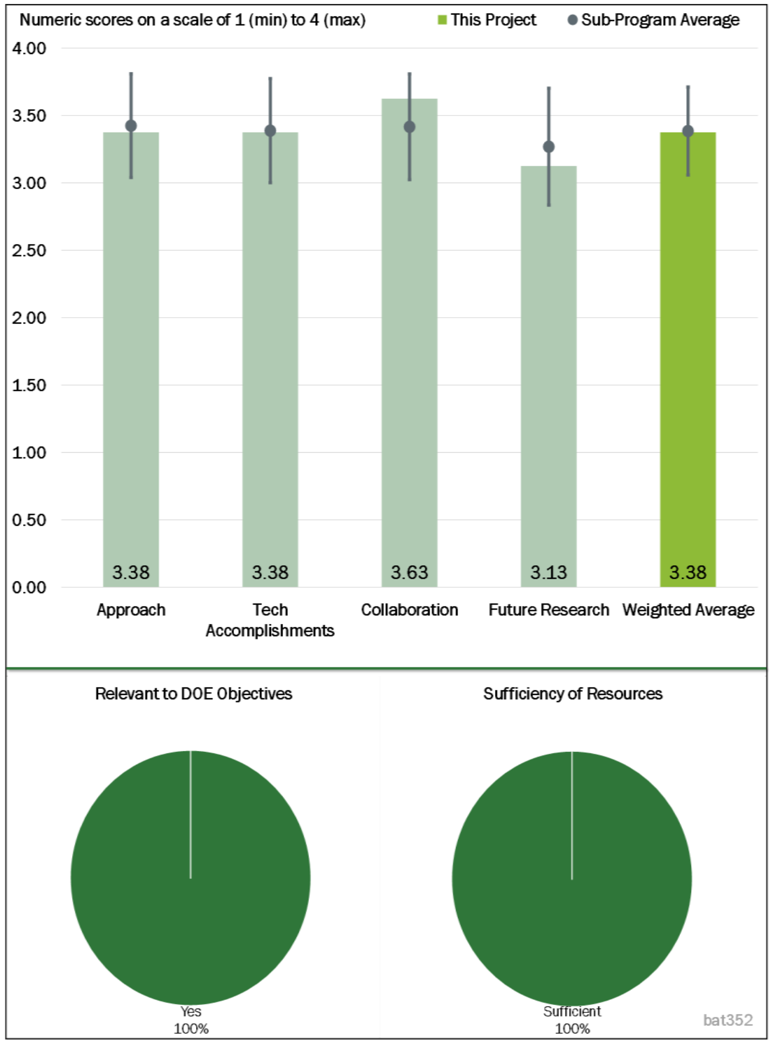

Figure 2-54 - Presentation Number: bat352 Presentation Title: Active Materials Advancements Principal Investigator: Zhengcheng (John) Zhang (Argonne National Laboratory)

Presenter

Zhengcheng (John) Zhang, 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 and well-planned.

Reviewer 1:

The reviewer commented that the group is synthesizing a myriad of Si materials, each with its own unique means of improving cyclability, to understand the benefits of different configurations.

Reviewer 2:

The reviewer said that a variety of approaches are used apparently to elucidate the effect of particle morphology. The reviewer recommended that some outline of the objectives and long-term goals would be useful.

Reviewer 3:

The reviewer said that the Si advanced anode materials optimized for swelling will improve the life of the Li-ion cells

Reviewer 4:

With so many techniques have been applied in this project, the reviewer thought the approach was well-outlined, difficult but feasible, and aligned with other focuses in this big Si program. The reviewer said that if successful, the effort will result in a successful application of a Si anode in next-generation high-energy Li-ion batteries.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer pointed out that a lot of data have been generated; some of it duplicates previous data reported by these groups and other national laboratories. A one-page summary of current conclusions and new contributions to the understanding of Si anodes would be helpful.

Reviewer 2:

The reviewer noted that there are enormous works focused on Si/SiO modifications in this project, which are vital to enable high-capacity Si anodes in next-generation Li-ion batteries. The reviewer pointed out that the electrolyte and additive work related to SEI formation is another key factor to enable a Si-based anode. The reviewer believed this project is on the right track and made great progress in this period.

Reviewer 3:

The reviewer said that the team synthesize a number of materials, provide a schematic of what was made, and then provided good evidence that what was made was what the team hoped to make. The reviewer pointed out that the team then provided testing data with comparable chemistries. The reviewer was unsure why the team show cycling against Li but not a lot of cycling in a full cell, and was unsure how the team assessed CE when there is capacity fade.

Reviewer 4:

The reviewer said that the cycle life test should be continued for more than 1,000 cycles before concluding on the stability of Si anode, and the charge profile should include the fast charge requirements.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that collaboration and coordination among six national laboratories is great for this big program.

Reviewer 2:

The reviewer remarked excellent collaboration is working among the DOE national laboratories.

Reviewer 3:

The reviewer said that there is an extensive collaboration between participants in the project.

Reviewer 4:

The reviewer observed a lot of synthesis, a lot of SEMs, a lot of spectroscopic data, and a lot of cycling data. The reviewer said that this takes a lot of collaboration.

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

Reviewer 1:

The reviewer said that the proposed work is interesting. It would be good to establish the role of the C/Si interactions.

Reviewer 2:

The reviewer said that there are so many good future research directions for this program. The reviewer would like to know whether all the partners in this program can use the same baseline materials from CAMP, which can make the comparison of performance improvement much clearer. The reviewer also said that an impedance study is also a good tool to evaluate different Si materials performance, which may deserve a more important role for the future research in this program.

Reviewer 3:

The reviewer said that future optimization should be aligned to the lifecycle of more than 1,000 cycles and fast-charge capability of 4C charge rates.

Reviewer 4:

The reviewer was unclear how the team selected the materials that are going to be pursued next. The reviewer said that it would be nice to see some of the diagnostics and efforts from SEISta have some influence on the selection.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer remarked that development of high-energy cells with Si-based anodes is a great support for DOE objectives.

Reviewer 2:

The reviewer agreed that the work is relevant to the development of high-capacity anodes.

Reviewer 3:

The reviewer commented that figuring out how to get Si to cycle certainly supports DOE objectives of increasing energy density.

Reviewer 4:

The reviewer remarked that the optimized electrode material will increase the sp. energy, energy density, and life of the 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 said that resources are sufficient.

Reviewer 2:

The reviewer found that $3.6 million should be sufficient to support the work described here.

Reviewer 3:

The reviewer said that the facilities and resources are excellent.

Reviewer 4:

Like every presentation given in this block, the reviewer had no clue how much this group receives relative to any other group. Apparently, there is no oversight of how funding is distributed.

Presentation Number: bat353
Presentation Title: Crucial Supporting Materials Advancements
Principal Investigator: Gao Liu (Lawrence Berkeley National Laboratory)

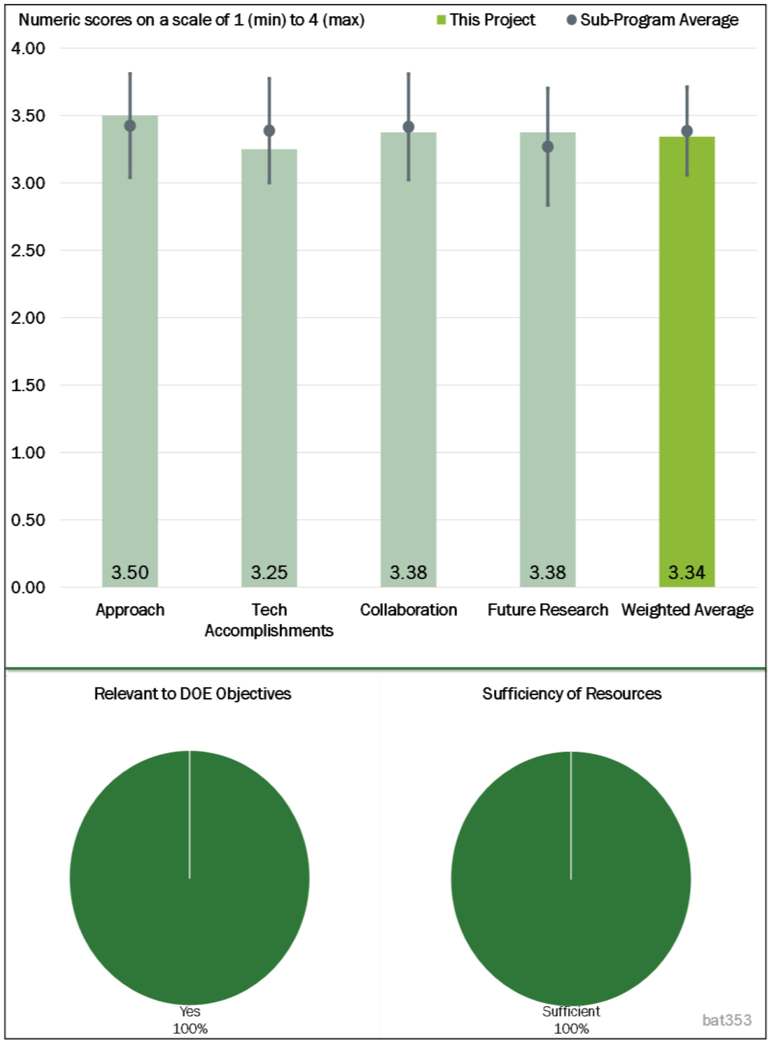

Figure 2-55 - Presentation Number: bat353 Presentation Title: Crucial Supporting Materials Advancements Principal Investigator: Gao Liu (Lawrence Berkeley National Laboratory)

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 and well-planned.

Reviewer 1:

The reviewer appreciated the systematic approach taken by the investigators. The team appeared to start from a baseline chemistry and build on it as the team learned how it was performing.

Reviewer 2:

The reviewer pointed out that identifying additives, binders, and pre-lithiation techniques to increase the cycle life and reduction of swelling will help DOE to meet its energy goals.

Reviewer 3:

The reviewer observed an excellent approach by combining of the development of electrolyte additives, electrode binder, and Li inventory to support this Si anode program.

Reviewer 4:

The reviewer said that the proposed approach is very appropriate. Because a lot of work has been done inside and outside the program, comparison to previous reports on this topic should be essential.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that the project team is investigating several ways to improve the cycling of Si and understand effects in full and half cells. Once a material is tested, the team makes systematic changes to improve it.

Reviewer 2:

The reviewer commented that all the technical accomplishments are still in early stage; most investigations are focused on understanding the mechanisms between Si and other components in the cell. The reviewer saw a lot of progress in this project, especially the Li inventory part, and really wants to see the difference among various cathode materials. The reviewer noted that if this study can be successful in the near future, the application of Si material in a high-energy system can be really facilitated.

Reviewer 3:

The reviewer pointed out that further research on identifying optimized additives, binders, and pre-lithiation strategies will lead the cell development to meet DOE goals.

Reviewer 4:

The reviewer noted that the project has generated a lot of data, and the study of binders seems interesting and useful. The reviewer suggested that more integration with the other (BAT350, 351, 352) projects would be useful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted that there are researchers thinking of new chemistries, others making new chemistries, others scaling up new chemistries, electrodes being fabricated, and cells being tested. The reviewer concluded a well-coordinated team.

Reviewer 2:

The reviewer noted that coordination and collaborations are very good.

Reviewer 3:

The collaboration among the national laboratories will lead to improved life of Li-ion cells.

Reviewer 4:

The reviewer said that more interaction with the other teams is desirable, so the project can accomplish the stated objectives.

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 remarked that the additives, binders, and pre-lithiation will play a critical role in Li-ion cell improvements.

Reviewer 2:

The reviewer remarked that the proposed study of binders and additives could be key for the stabilization of the anode.

Reviewer 3:

The reviewer observed well-designed proposed future research with a lot of detailed information. This is really helpful for handing such big program with so many collaborators.

Reviewer 4:
The reviewer commented that there are a lot of materials being considered, some new, some improvements of others. The reviewer expressed uncertainty why so much work is needed in pre-lithiation. This is not the problem; consumption of Li with cycling is. The reviewer stated we know how to do pre-lithiation.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer found that the project supports DOE's objective of developing high-capacity anodes.

Reviewer 2:
The reviewer believed the development of Si anode materials is super important for the next-generation high-energy Li-ion batteries. The electrolyte and additive development is a key factor to enable Si materials and deserves much more attention than it currently has.

Reviewer 3:
The reviewer remarked that success in this project will help with getting more Si in the anode to improve capacity density and thereby energy density.

Reviewer 4:
The reviewer said that the reduction in swelling and improvement in electrode behavior will help to meet DOE goals.

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

Reviewer 1:
The reviewer remarked resources and facilities are excellent.

Reviewer 2:
The reviewer said resources are sufficient.

Reviewer 3:
The reviewer stated that DOE resources for the R&D work are sufficient.

Reviewer 4:
The reviewer said no clue, and that one giant number was given for the entire project.

Presentation Number: bat355
Presentation Title: Development of High-Performance Lithium-Ion Cell Technology for Electric Vehicle Applications
Principal Investigator: Keith Kepler (Farasis Energy)

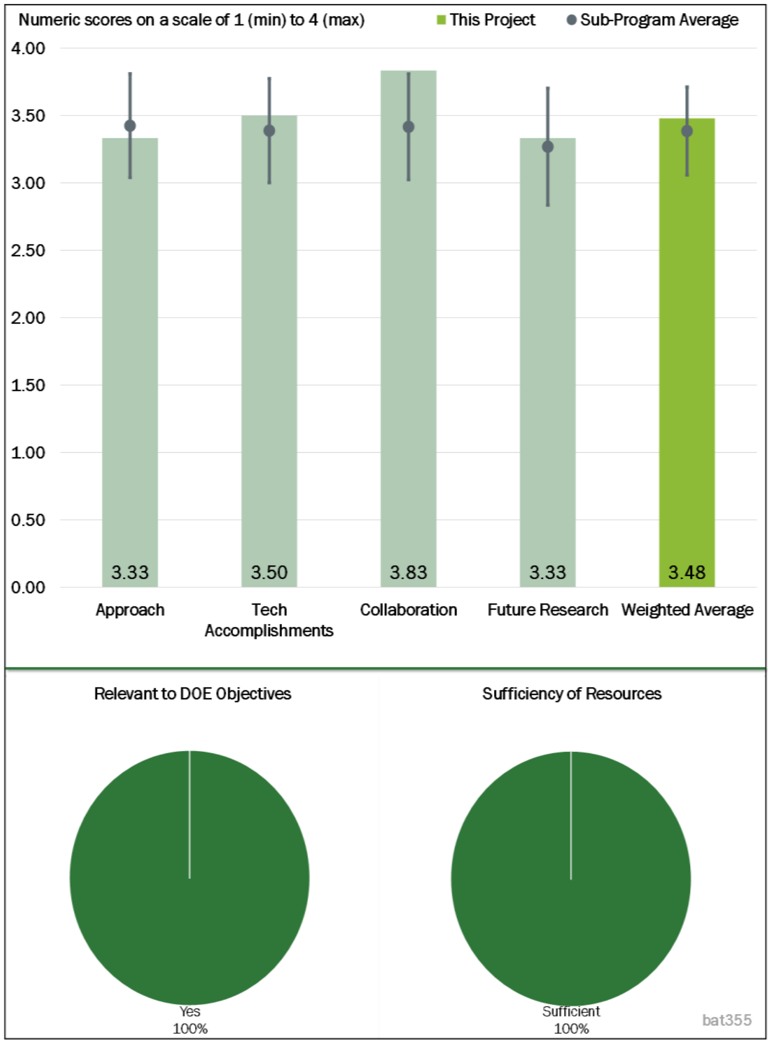

Figure 2-56 - Presentation Number: bat355 Presentation Title: Development of High-Performance Lithium-Ion Cell Technology for Electric Vehicle Applications Principal Investigator: Keith Kepler (Farasis Energy)

Presenter

Madhuri Thakur, Farasis 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 and well-planned.

Reviewer 1:

The reviewer said that although the electrode active material couple is not novel, the project is addressing many challenges related to successfully implementing Ni-rich cathodes and Si-C anodes for long-term performance, such as stabilizing the anode and cathode SEI layers. This project is well-designed and laid out given that there are so many variables and test matrix materials. The reviewer said the project has clear milestones and deliverables, and relevant pouch cell cycling performance evaluation. The reviewer expressed as a concern the impedance problems at the cathode with the Li-iron oxide source, but there is a clear plan in future work to understand this phenomenon. The reviewer said that it would be good to see calendar life testing as part of the future work for this/these electrochemical couple(s).

Reviewer 2:

The reviewer detailed that the project aims to address the key barrier to achieve high-capacity, long cycle life, and safer Li-ion cells. The reviewer summarized that Li-ion battery performance is improved via developing high voltage (≥ 4.6V Ni-rich/Mn-rich cathode composites, high-performance Si-based anode, and fluorinated solvents and stabilizing additives/salts for the electrolyte. The composition and structure of both anode and cathode materials are not described. The reviewer was unclear what specific strategy has been devised to realize the goal of project.

Reviewer 3:

The reviewer detailed that the proposed approach integrates a high-energy cathode, Si composites, and optimized electrolyte into pouch cell format for evaluation. The Li source materials are also validated in cathode. The reviewer said that although the PI mentioned a target on the cell-level energy when screening the cathode and anode, it is not clear what the specific areal capacities of both cathode and anode need to reach. In addition to the specific capacity of active materials, the electrode-level porosity, electrode press density, etc. all play key roles in determining the cell-level energy. The reviewer said that the PI needs to provide a number of areal capacity and mass loading that all the research will be built on.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that there has been a significant amount of progress, especially for a new start, on all major technical categories. However, the anode conductive additives do not seem to improve performance over the control cell.

Reviewer 2:

The reviewer said that the investigators have finished the evaluation of the high Ni-content based cathodes and different materials options for Si anodes and the optimized electrolyte. The high-energy cells exhibit energy density of greater than 300 Wh/Kg. The reviewer said that the cyclic testing data should be provided, and the slides should give a detailed description of the difference of the developed anode and cathode from those previously reported.

Reviewer 3:

The reviewer said that the team has evaluated 12 cathodes, 4 anodes and down-selected A1 and C1 for a Gen1 deliverable. Electrolytes and C additives are also evaluated to improve the cell performances. The reviewer was unclear how much Li resource needs to be used in Gen 1. To get a maximum utilization of the anode materials, the percentage of Li source in the cathode will be adjusted to compensate the first cycle loss. However, it is unknown what the ratio of negative to positive electrodes (N/P) is in the Gen 1 cell. The reviewer said that incorporating a sacrificial source in the cathode adds on more “parasitic.” weight and sacrifices the cell-level energy. The reviewer was unclear how the team will balance the cell energy and first cycle loss. The single or double layer pouch cells are tested in flooded electrolytes. The reviewer asked if the author calculated how much electrolyte will be actually incorporated the in Gen 1 cell. If the single or double layer pouch cells are tested under such lean electrolyte conditions, the reviewer asked whether the cycling will last for the same few hundreds of cycling.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that collaboration with ANL and LBNL have benefited the project.

Reviewer 2:

The reviewer pointed out that ANL’s contribution is quite clear in this project, i.e., to develop a sacrificial Li-source for Si anode. The reviewer noted that LBNL is helping on the high-voltage conductive additive for this project.

Reviewer 3:

The reviewer said that collaboration is outstanding in this project. The PI has covered active material suppliers, inactive material suppliers, cell manufacturing, and strategic national laboratory partners. However, the manufacturing scale-up process was not adequately discussed, which would presumably be handled by Farasis. The reviewer asked if there are any other partners needed for this portion.

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

Reviewer 1:
The reviewer said that in the future work, the team will focus on delivering Gen1 Cell and the Gen 2 Development, which is logically planned according to the overall objectives of the project. For the Gen 1 cell, the project will target high capacity of specific energy of ~ 300 Wh/Kg, energy density of ~ 625Wh/L, a long cycle life of greater than 500 cycles, and safety, which are the key barriers and issues for current Li-ion batteries. However, the reviewer said that the investigators should describe their approaches as well as the composition and structure of both the cathode and anode in detail.

Reviewer 2:
The reviewer said that the team will deliver a Gen1 cell with 300 Wh/kg (625 Wh/L) of energy and greater than 500 cycle life this year. The team also proposed a plan to develop the Gen2 cell. From 330 Wh/kg to 360-375 Wh/kg, it seemed to the reviewer that the same C2 materials will be used while the anode will be changed from A1 to A2. The reviewer was unclear why the cell energy can be boosted to greater than 360 Wh/kg simply by changing the anode composite. The reviewer commented that if there is no further reduction on the porosity (of both electrodes) and other parasitic weight, it is not feasible to improve cell energy by only increasing anode capacity.

Reviewer 3:
The reviewer suggested adding calendar life testing, manufacturing scale-up, and electrode design parameters (i.e., areal capacity targets).

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that this project takes an important step of making commercially available materials work at stressful operating conditions to substantially increase cell gravimetric energy density to well over 300 Wh/kg. The technology has a high likelihood of commercialization and a strong intellectual property position. The reviewer said that it also places the domestic Li-ion battery supply chain in a much stronger position as compared to the international competition.

Reviewer 2:
The reviewer said yes, and elaborated that the on-going research will facilitate DOE's goal to improve the energy density, power density, and cyclic performance.

Reviewer 3:
The reviewer remarked that this project is to develop an EV cell technology capable of providing 350 Wh/kg for 1,000 cycles at a cost target of $0.10/Wh. The reviewer found that this goal is well-aligned with DOE/EERE/VTO 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 said that the resources for the synthesis and characterization for experiments are sufficient for the project.

Reviewer 2:

The reviewer said that this project is a large effort, and a $5.9 million award (with 50% cost-share) is in line with all of the materials screening, electrode optimization, cell optimization, and process scale-up R&D that will need to be done. However, this reviewer questioned if all the milestones and metrics can be completed by September 2019.

Reviewer 3:

The reviewer commented that the PI has subcontractors with two different national laboratories which both have sufficient resources to conduct the proposed work from materials research to pouch cell preparation. The team also has many industry partners to aid the R&D.

Presentation Number: bat356
Presentation Title: Lithium-Ion Cell Manufacturing Using Directly Recycled Active Materials
Principal Investigator: Mike Slater (Farasis Energy)

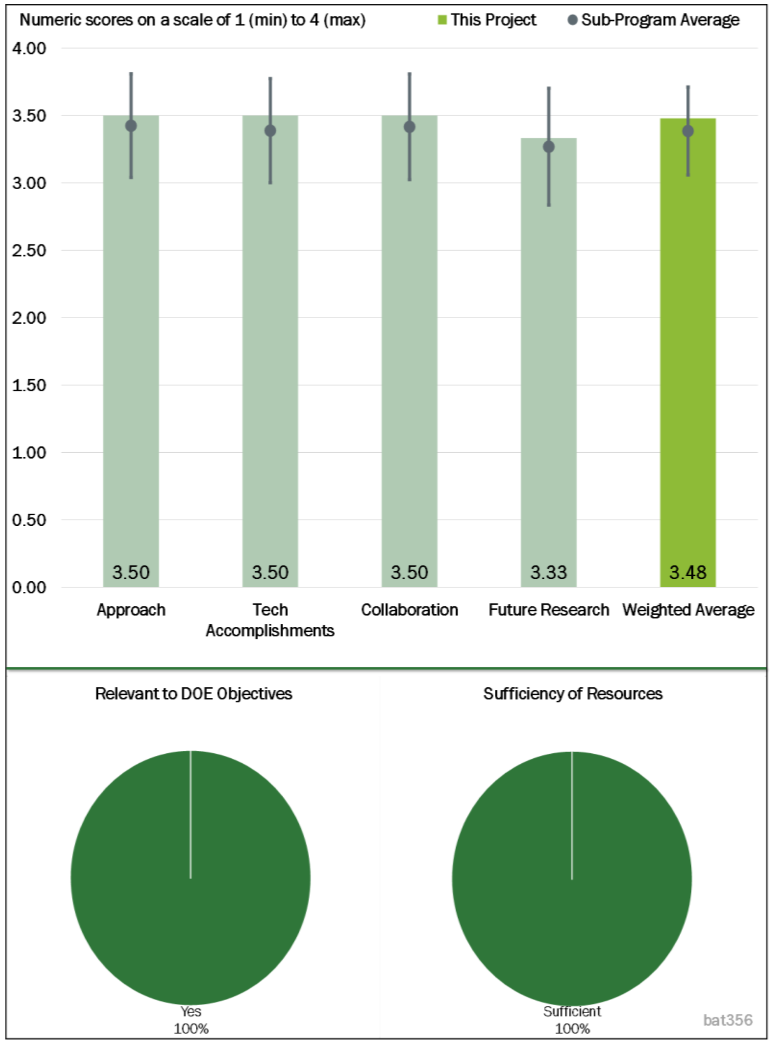

Figure 2-57 - Presentation Number: bat356 Presentation Title: Lithium-Ion Cell Manufacturing Using Directly Recycled Active Materials Principal Investigator: Mike Slater (Farasis Energy)

Presenter

Mike Slater, Farasis 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 and well-planned.

Reviewer 1:

The reviewer commented that a direct recycling method is used to obtain recycled materials from discharged cells. The physical separation process is used for low-cost value recovery of wastes from the used batteries. The reviewer pointed out that an intermediate cell has been built with recycled active materials, which provides the data for quantitative technology valuation. The reviewer found that the project is well designed and feasible.

Reviewer 2:

The reviewer said that this project is well-designed and addresses all outlined technical barriers. The reviewer said that more emphasis should be placed on recycling of long-term tested cells (rather than the assumption made that 10-year old active materials perform the same as recycled ones), although the proposed direct recycling pathway for non-formed cells seems applicable to all cases. The reviewer remarked that the all-physical separation process is particularly interesting and elegant, but adding in the thermal treatment step to the process flow diagram would be helpful.

Reviewer 3:

The reviewer said that direct recycling of cathode and anode materials from spent Li-ion batteries is proposed with some preliminary results demonstrated. Physical separation processes are used to recover active materials while chemical purification and re-lithiation are proposed to be performed under mild conditions. The reviewer's main concern of the proposed approach is to ensure the fully restored Li inventory in each different NMC resource. Residual Li in NMC could vary significantly from each different recycled battery. The reviewer suggested that a method to predetermine Li inventory in the cathode is needed. The reviewer was not clear how to "regenerate" the cathode by adding more Li into the lattice structure. The majority of the proposed approach is based on the assumption that the pouch cells have already been successfully built by using the recycled materials.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that facility modifications were completed last year, capable of recycling active materials several kilograms per day. The project investigated thermal treatment of both the positive electrodes and negative electrodes. The reviewer pointed out that results show increasing the processing temperature increased the purity of recovered metal oxide but diminished the recovery of Gr. The project created and extended a process model for direct recycling, which helps optimize the recovery processes. The reviewer found that the progress is on track to realize the overall objective.

Reviewer 2:

To the reviewer, it seemed as though several of the key milestones are delayed and many have not yet been met, but the project is designated as 66% complete. The reviewer found that overall, good technical progress has been made, especially the cathode post-thermal-treatment capacity and Raman spectroscopy results. This reviewer is curious if the PI has considered the tradeoffs between anode thermal treatment temperature effects on Gr oxidation and removing SEI components. The requirements of Gr yield and SEI layer removal seem to be in competition with each other.

Reviewer 3:

The reviewer said that the project has studied the thermal treatment effects on cathode and anode recycling, and demonstrated the materials separation. However, there are quite a few important milestones delayed.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer pointed out that the company teams up with LBNL by using their characterization facilities.

Reviewer 2:

The reviewer noted that more collaborators than just LBNL will likely be needed for the extensive materials characterization that will be required to address the material complexity issues the PI identified.

Reviewer 3:

The reviewer said that this project is performed through the collaboration with LBNL. The collaboration helps chemical diagnostics and materials characterization to guide recycling process 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 found that the future work is well-planned. The team will extend a direct recycling process to additional formed cells and complete modules feedstocks; complete cell construction, and gain understanding of the impact of recycled materials on technology lifetime.

Reviewer 2:

The reviewer recommended that the challenges and barriers slide needs to be expanded for more granularity. The proposed future research addresses the major open challenges with the exception of retesting long-term-cycled recycled active materials (although it is at least addressed in the assumptions section). The reviewer said that it would be interesting to see, for example, how active materials perform that are tested for 1,000 USABC cycles, which are then recycled and retested for another 1,000 cycles. This reviewer recognized the length of time involved with that plan, and it may be beyond the scope of the given timeframe. The reviewer pointed out that it will be difficult to finish this project by January 2019, and an extension may be needed.

Reviewer 3:

The reviewer said that proposed future research will extend the direct recycling process to form cells and complete modules. Without successful delivering the cells consisting of recycled materials, it is too early to extend the process to modules and other cell chemistries. The reviewer said that the team needs to identify the key fundamental challenges of direct recycling process and address them first before rushing into building cells or modules. The reviewer said that a clearer techno-economic model is needed to understand the cost for the proposed recycling process and its impact.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said yes, and elaborated that implementation of this project will lower the costs for battery production and reduce the environment pollution of the disposed batteries.

Reviewer 2:

The reviewer said that direct recycling of active materials from spent batteries are relevant to DOE/VTO objectives.

Reviewer 3:

The reviewer said that recycling cathode active materials is critical to meeting VTO’s new low/no Co goals. Recycling anode and cathode active materials should significantly reduce cost, as the recycling costs will be less than the synthesis cost of pristine materials. The reviewer found that this project will help in achieving VTO’s ultimate cost target of $80-$100/kWh.

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 the facilities and characterization for experiments are sufficient to achieve the goal of the project.

Reviewer 2:

The reviewer said that Farasis has the ability to build cells while LBNL has resources for characterization and materials testing.

Reviewer 3:

The reviewer said that $1.8 million for this project is reasonable, but it would be interesting to know how much has been spent to date relative to the milestone progress.

Presentation Number: bat357
Presentation Title: Thicker Cathode Coatings for Lithium-Ion Electric Vehicle Batteries
Principal Investigator: Stuart Hellring (PPG Industries)

Presenter

Stuart Hellring, PPG Industries

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 and well-planned.

Reviewer 1:

The reviewer said that this project is highly relevant and feasible, as thick coatings for lower cost and higher energy density are important. However, there is no plan in this work on how to address the high-power limitations of these coatings (i.e., 5-9 mAh/cm^2). The reviewer also commented that no details were provided on how to switch from the solvent system (which is of limited benefit over conventional NMP to a pure water system.

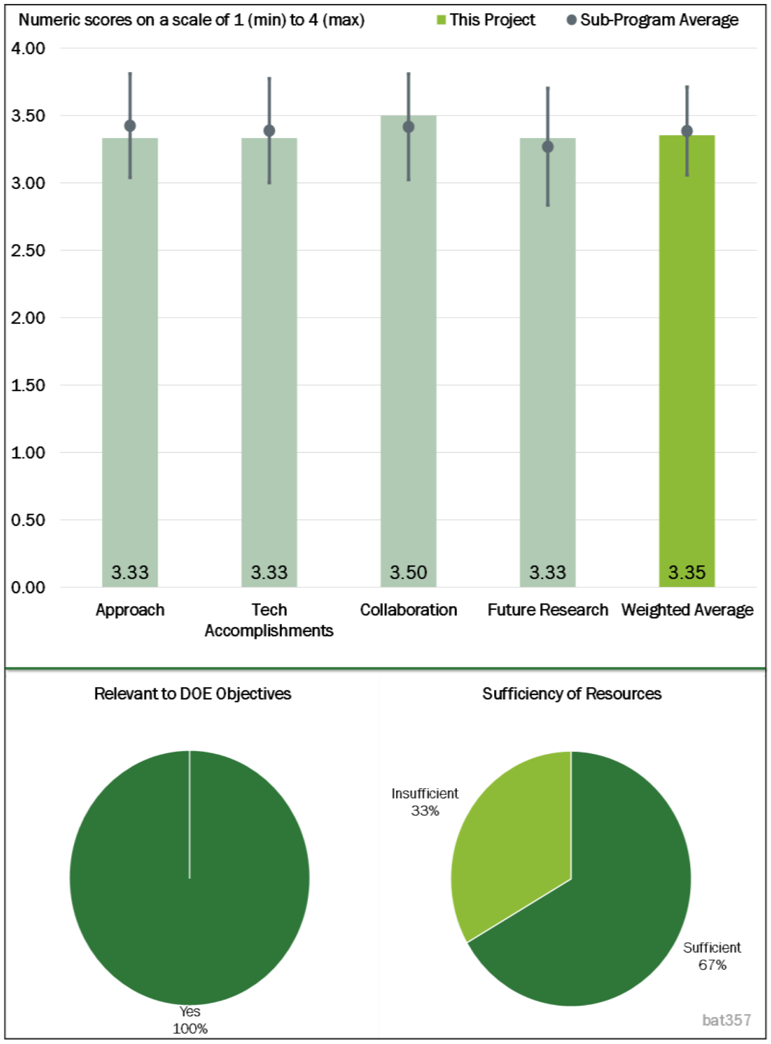

Figure 2-58 - Presentation Number: bat357 Presentation Title: Thicker Cathode Coatings for Lithium-Ion Electric Vehicle Batteries Principal Investigator: Stuart Hellring (PPG Industries)

Reviewer 2:

The reviewer commented that the project is to address the critical barrier of a low-area density electrode, which limits the overall energy density. The project is designed to investigate the NMP-free cathode. This approach will increase the environmental compatibility of the cathode manufacturing. The reviewer said that the thick film performance will be improved by optimizing processing conditions, and battery size/weight/cost will be investigated. The PPG binder has some advantages over the NMP binder. However, the reviewer was unclear why the PPG binder is better than the NMP binder. The composition and the properties of the PPG binder are unclear. It is unclear why the PPG binder-based cathode can be thick without sacrificing the power density and cyclic performance. In other words, the reviewer thought that the reason for enabling thick cathodes should be described clearly and justified.

Reviewer 3:

The reviewer said that this project develops an NMP-free solvent to make thick cathodes with good flexibility without sacrificing the electrochemical properties. High areal capacity is beneficial to improve cell energy. However, increasing cathode loading/areal capacity without further reducing the electrode porosity will have limited impacts on the energy increase. The reviewer recommended that the project needs to calculate the cell-level energies that the team would like to reach by using different thicknesses of electrodes instead of simply increasing the cathode loading. Electrolyte intake will also increase proportionally if the cathode becomes thicker lowering the cell-level energy. The reviewer said that the percentage of NMC in the electrode needs to be increased to 96% or above to further increase the areal capacity. The reviewer asked if the minimum amount of PPG binder is 4%, or it can be further lowered.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:
The reviewer noted the project achieved a greater than 5.3 mAh/cm^2 areal capacity and passed mandrel test with good quality. Thick electrodes are tested in pouch and cylindrical cells with some discrepancy though. The reviewer said that final goals have been reached, and the team will develop a matching anode to build cells.

Reviewer 2:
The reviewer observed excellent progress on the processability of the thick cathodes, but much work on the anode and rate performance metrics still needs to be done. It seems as though the team is having trouble with continuity of full cell builds as well.

Reviewer 3:
The reviewer said that the PPG binder has been used to manufacture a high area-density cathode, reached up to 145 um per side for the double-sided coating with pilot-scale R2R coater, up to 40 mg/cm^2 mass loading. The reviewer said that the cathode coatings exhibited good flexibility and peel strength (90°), exceeding 66N/m to meet final target specification. However, the reviewer thought the use of “NMP-free binder” is confusing. In fact, it is not a binder-free cathode. Instead, the PPG binder is used to replace the NMP binder

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said great collaboration throughout the whole team, including industry, a national laboratory, and universities.

Reviewer 2:
The reviewer said that this project is performed through collaboration with LG Chem Power, Idaho National Laboratory (INL), and PSU.

Reviewer 3:
The reviewer inquired why there are so many partners for full cell testing. It seemed as though PPG could benefit from spreading the activities better throughout the team.

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

Reviewer 1:
The reviewer detailed that future research is to develop a high-capacity electrode with a thicker coating, and further optimize electrode pairs toward final deliverables. Also, the team will apply and optimize the PPG binder for high Ni active materials. The team is also planning water stable active materials.

Reviewer 2:
The reviewer pointed out that the team has already accomplished the final target. The team is trying to develop a thick anode to match the cathode. In addition to the work the team proposed, other modifications are also needed. The reviewer detailed that the percentage of NMC is 93%, which is less than what industry cells

usually use, i.e., 96% or higher. The reviewer asked if there is a reason that the PPG binder needs to be 4% in the electrode fabrication. Porosity control is more challenging in thick electrode but more meaningful for improving cell-level energy than just making thicker electrodes. The reviewer said that the team needs to consider how to control the porosity and tortuosity of the thick electrodes in order to reach the same good electrochemical performances in thicker but denser electrodes.

Reviewer 3:

The reviewer said that the proposed future research is weighted too heavily on the processability of the thick electrodes. The reviewer commented there is not enough emphasis on performance limitations that these types of electrodes must overcome at high discharge rates. The processability and performance need to be approached holistically. Also, the reviewer pointed out that there are not enough details on how the pure water stability of the cathode materials will be characterized and addressed.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer commented that the thick electrode with high areal capacity will boost the cell-level energy, and is directly relevant to DOE/VTO objectives in developing high-energy EV batteries.

Reviewer 2:

The reviewer said yes. If successful, the outcome of the project will reduce the overall battery cost and size/weight, and improve safety during the manufacturing process.

Reviewer 3:

The reviewer said that the thick electrode coatings are highly applicable to achieving the ultimate VTO cost target of $80-$100/kWh, and the ultimate gravimetric energy density target of 500 Wh/kg.

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 in order to address what this reviewer considered as the process-property-performance gap in this project, it is underfunded.

Reviewer 2:

The reviewer said that the resources are sufficient to achieve the goal of project.

Reviewer 3:

The reviewer said that the University of Michigan has the pouch cell facility, LG Chem also participates in the pouch cell preparation and testing, Penn State is working on matching anode, while Coulometrics works on cathode coating. The reviewer said that the role of INL seems to be overlapping with other team members.

Presentation Number: bat358
Presentation Title: Advanced Separators for Vehicle Lithium Battery Applications
Principal Investigator: Junqing Ma (Celgard)

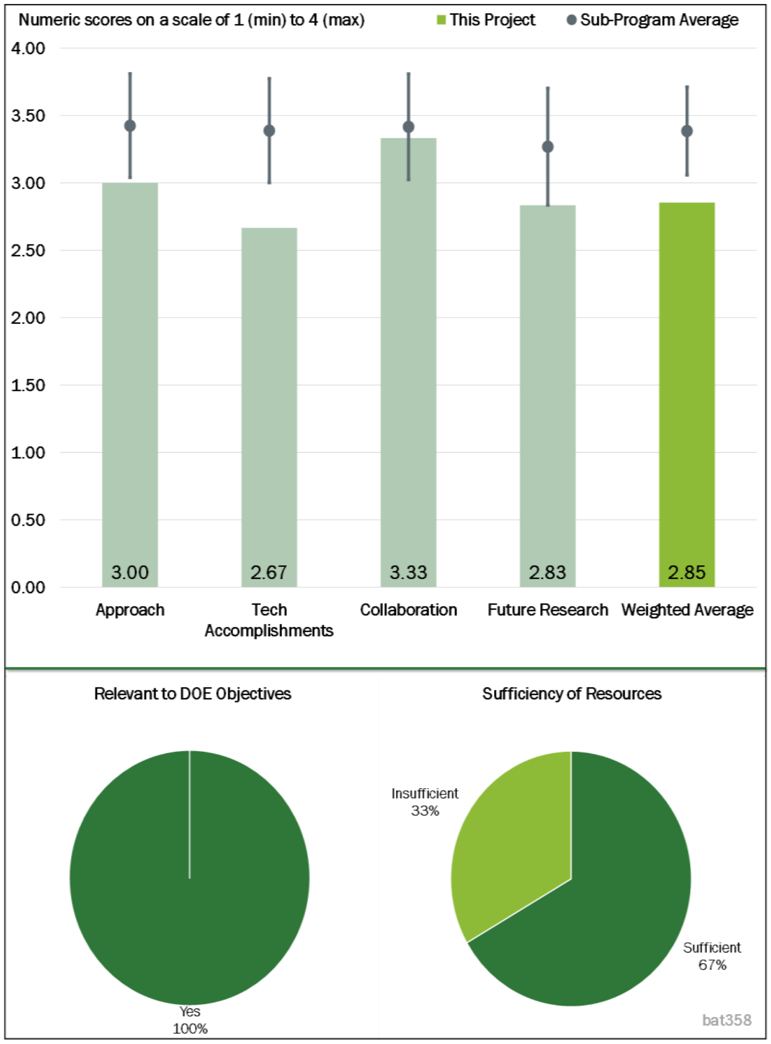

Figure 2-59 - Presentation Number: bat358 Presentation Title: Advanced Separators for Vehicle Lithium Battery Applications Principal Investigator: Junqing Ma (Celgard)

Presenter

Junqing Ma, Celgard

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 and well-planned.

Reviewer 1:

The reviewer said that the approach is feasible and addresses relevant technical barriers, but this reviewer does not believe the project addresses the main challenges associated with 5V systems. The reviewer noted that the electrolyte and the cathode surface stability are far more critical to overcoming this barrier. It seems as though the project considers these aspects, but the lead is a separator developer.

Reviewer 2:

The reviewer detailed that the project aims to develop a separator with high voltage stability in 5V cells, and a nanometer-scale ceramic coating on the separator to enhance the resistance to electrochemical oxidation. After the conformal ceramic is coated and the polymer composite separator is produced, the 5V cells will be used to test the cycling and stability of the separator. However, the rationale for the separator design is not described. The reviewer elaborated that the chemical composition, chemical structure, and microstructure are unclear. The specifications and properties of separator are also unclear, and the method for separator evaluation is not described. The reviewer said that the advantages of the proposed separator over the current separators need to be described.

Reviewer 3:

The reviewer detailed that Celgard will fabricate protected separators that can tolerate 5V for high-energy batteries. The separators will be tested in the pouch cell provided by Farasis. However, the reviewer did not know what kind of coating materials or method will be used to enable the high-voltage operation stability of separators. The reviewer said that fundamental knowledge and a roadmap are lacking in this project.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that the project is over a year old and only one Technical Accomplishments slide was given with no data. The first major milestone was at least met by providing five ceramic coated separators to Farasis.

Reviewer 2:

The reviewer summarized that five ceramic coated separators and several polymeric composite separators have been fabricated and characterized. The first-generation 5V cells showed encouraging capacity and cycling performance. The reviewer pointed out that the team identified issues for capacity fading including cathode dissolution and electrolyte degradation. However, the chemical composition, chemical structure, and microstructure need to be described, and details on the capacity and cycling testing need to be provided. The reviewer recommended that targeted performance metrics should also be provided.

Reviewer 3:

The reviewer pointed out that there is only one page summarizing the accomplishments to date, although the project started more than one year ago. The reviewer reported Celgard fabricated and five ceramic coated separators were characterized, to which this reviewer asked what they are; what the characterization results are; and how they are expected to differ from other coatings and tolerate high voltage. No figures or experimental results are provided, which made the review process hard for this reviewer. Further, this reviewer dropped by three times during the poster session, but no one was there answering questions.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that this project is performed through the collaboration with Farasis Energy and ANL.

Reviewer 2:

The reviewer noted that a lean, but strong team has been assembled in Farasis, ANL, and Celgard. The reviewer clarified that Farasis is a reliable partner for the full cell testing, and ANL will handle the cathode powder coatings for achieving a cell voltage of 5V.

Reviewer 3:

The reviewer detailed that Celgard teams up with Farasis Energy and ANL. Farasis will provide 5V cell design and evaluate 5V cell cycling performances and fabricate cells.

The reviewer said that ANL will do coating work to enhance the cathode stability at high voltages. The reviewer said that no results were provided from the partners in the slides.

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

Reviewer 1:

The reviewer said that Celgard will work with Farasis and ANL on down-selecting fabricated separators and developing protected cathode materials to address the issues identified in earlier 5V cells fabricated by Farasis. The reviewer detailed that future research also includes the evaluation of the stabilized 5V cells based on cycling and storage stability and finalizing the design for 12-month deliverable cells.

Reviewer 2:

The reviewer found that the plan to meet the goals of fabricating a separator that can operate at 5V is not clear. The reviewer said that simply down-selecting from the fabricated separators is not a good plan; what if none of them work. Without a fundamental understanding and a clear strategy to address the challenges, it is not promising that the project will meet the final goals.

Reviewer 3:

The reviewer detailed that the most important aspects of 5V systems (electrolyte and cathode surface stability) were identified as both remaining challenges and needed future work, but it is not clear to this reviewer what role Celgard will play in overcoming those barriers. Therefore, the project, may need to be re-scoped for the remaining 2 years.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said yes, 5V systems are an important mark to hit for achieving VTO’s ultimate gravimetric energy density target of 500 Wh/kg. The reviewer is of the opinion that this project is not working on the most important aspects to achieving 5V, however.

Reviewer 2:

The reviewer said that the slides/report should describe the reliance of project.

Reviewer 3:

The reviewer said that improving separator stability at high voltages is relevant to VTO needs. This reviewer was not quite sure why there is a need for high voltage at 5V though.

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 $2.5 million over 3 years is adequate for this project and meeting the key remaining milestones.

Reviewer 2:

The reviewer said that the resources are sufficient to achieve the project goal.

Reviewer 3:

The reviewer commented that the PI mentioned in the “Remaining Challenges and Barrier” slide that “Full evaluation/understanding of separators degradation requires extended time and resources.” Although the reviewer believed a national laboratory should have most of the required resources to conduct the fundamental research, the team seems to think their current resources are insufficient.

Presentation Number: bat359
Presentation Title: Status and Challenges of Electrode Materials for High Energy Cells
Principal Investigator: Stanley Whittingham (Binghamton University)

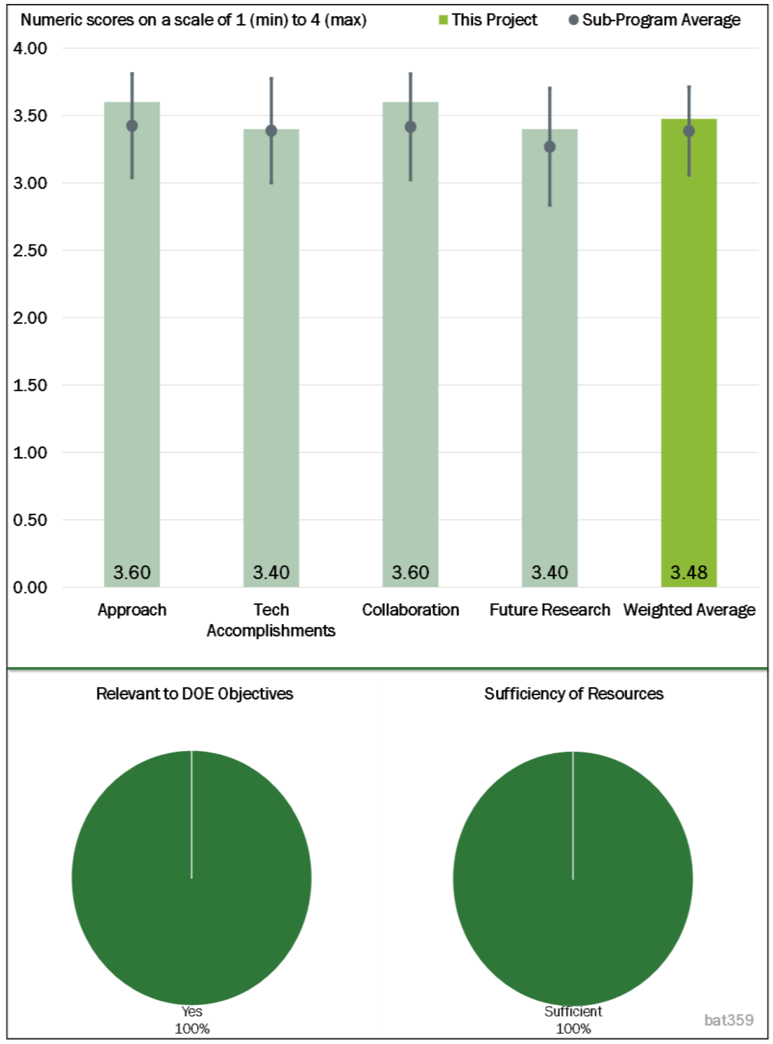

Figure 2-60 - Presentation Number: bat359 Presentation Title: Status and Challenges of Electrode Materials for High Energy Cells Principal Investigator: Stanley Whittingham (Binghamton University)

Presenter

Stanley Whittingham, Binghamton University

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 and well-planned.

Reviewer 1:

The reviewer said that the key barrier to achieve the Battery 500 objective is directly addressed in this project by focusing on the main bottleneck, i.e., the cathode. The approach rightfully calls for a dual-pronged development path—further enhance currently used and already mature layered cathodes and also develop the less-mature but potentially more energetic and less costly sulfur cathode. The reviewer said that the workplan is well-thought out and implementable.

Reviewer 2:

The reviewer commented that the problems of high-Ni NMC have been clearly defined, and they are being addressed. The team is starting with commercial material for baselines, which is the correct approach. The team will be looking carefully at optimizing structure/morphology.

Reviewer 3:

The reviewer said that the project is well-designed and feasible. The challenges of NMC and NCA are well addressed, and the pathway forward is presented well.

Reviewer 4:

The reviewer detailed that the goal of the overall Battery 500 project is to achieve a cell level specific energy of 500 Wh/kg through using a high-capacity cathode consisting of Ni-rich NMC or sulfur cathode, Li anode, and compatible electrolyte. The objective of this project is to evaluate cathode materials with different compositions in terms of rate capability and cycle life at different loadings, and make a recommendation to the project on future cathode compositions. The reviewer said that commercial NMC materials of compositions 622 (baseline) and 811 obtained different sources were evaluated in comparison with the NCA cathode and with materials synthesized by the Battery 500 PIs. There are several aspects still unknown with these Ni-rich materials including the role of Al in NCA, the effect of cathode loadings and coatings, and their degradation mechanisms, which are addressed in this project. The reviewer said that this project is well-designed and integrated with the other efforts under Battery 500.

The reviewer commented that with multiple teams working on the same materials, there is some confusion (and may be duplication as well) on who is doing what. Each of these groups (Binghamton University [BU], University of Texas-Austin [UT-Austin] and University of California-San Diego [UCSD]) have end-to-end capability to design synthesize, characterize and evaluate the new cathode materials, which made this reviewer wonder why there is this overlap.

Reviewer 5:

The reviewer was unclear why efforts were devoted to studying NCAs because the Battery 500 already committed to a Ni-rich NMC or S as the positive electrode and Li-metal as the negative electrode. Furthermore, the reviewer was unclear how the knowledge gained from studying NCAs can help solve much of the challenges facing NMCs because the two materials have different physical and chemical properties and degradation behavior.

The reviewer was unclear why the 622 and 811 NMCs obtained from the South Korea supplier were considered as baseline materials because their performance and durability appear to be worse than the commercial NMC811 by TODA America (see BAT164 presentation). The reviewer said that it may be helpful to exchange information with project teams outside the Battery 500 to select a baseline material.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that at the current stage, most of the work in the project is to characterize the baseline materials, which is presented well.

Reviewer 2:

The reviewer observed a significant amount of technical progress in the project. A number of studies involving baseline cathode materials, studies related to the role of Al in the stability of NCA, and air and thermal stability, among others, have been carried out prior to downselecting to the 811 cathode, which this reviewer described as a good selection.

The reviewer did have several comments, though. The authors have made general comments on air stability of several cathodes. As is well-known, this reviewer noted that property can also be tailored using a suitable coating. Additionally, making a statement on the cyclability of a certain material (in this case NCA, Slide 13) based on room temperature cycling up to 100 times can be misleading for material selection unless the difference in performance is quite significant, which it was not in this case. The reviewer opined that this begs the question of why one cannot cycle the cells at a higher temperature to accelerate degradation for easier materials differentiation.

Reviewer 3:

The reviewer observed an excellent job on characterizing commercial material. Studies of Li range in 622 and 811 are good, as are studies of Al. Many of the characterization measurements are not new, however. Of course, the project is still at an early stage. However, the reviewer expressed concern that the rate of progress is modest so far.

Reviewer 4:

The reviewer said that good progress has been made in characterizing and understanding the baseline NMC-622 material, which has been demonstrated in pouch cells (at PNNL), and in evaluating NMC-811 and NMC-900505 materials in comparison with the traditional NCA cathode. Compared to the baseline 622 cathode, 811 cathode gives higher capacity and better cycle life even at higher cathode loading and is of low cost and hence has been recommended for Battery 500 project. The reviewer said that when compared to the NCA cathode, which is well-studied and is routinely used in industry, the NMC 822 cathode has better air stability, less gassing, and high thermal stability. The role of Al is intriguing and seems to distribute uniformly in the bulk forming a solid solution and improving the cycle life.

The reviewer referenced prior comments, and noted that it is difficult to identify which group is doing what in this Battery 500 project, especially the manner in which the results are presented. There are some benefits in having good coordination in establishing future cathode materials for Battery 500, but with this much of overlap, there may be duplication and redundancy. The reviewer also pointed out that if these materials (622, 811) are already being commercially produced, the reviewer wondered what the rationale is, for DOE projects trying to synthesize/characterize these formulations. The reviewer said that instead, projects should focus other (new) formulations and with new coatings.

Reviewer 5:

The reviewer remarked that many of the learnings and recommendations are well-known in the literature, such as NMC 811 has higher capacity and higher power capacity. However, the reviewer asked if the manufacturing cost/kWh of NMC811 is lower than 622. Please carry out and report cost estimates.

The reviewer pointed out that the PDF presentation did not provide any evidence to support the statement that “Extended cycling leads to cracking of particles” (Slide 14). Also, the reviewer said that there is no evidence for keeping “lattice expansion to a minimum” to solve the cracking problem because a large strain does not necessarily lead to a large stress; e.g., many low modulus materials have low stress even at high strain.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that the collaboration among team members is outstanding.

Reviewer 2:

The reviewer said that the project has excellent collaboration among the team members.

Reviewer 3:

The reviewer observed good collaboration activities with the PIs in the Battery 500 projects, with researchers from PNNL, UCSD and UT-Austin, and also other DOE national laboratories. The reviewer suggested more active collaboration with industrial partners (e.g., TODA, Umicore, BASF, etc.).

Reviewer 4:

The reviewer remarked that the collaboration within the Battery 500 team seems strong. However, the team may benefit from collaborations with other DOE funded project teams, especially because many have or are working on Ni-rich NMCs.

Reviewer 5:

The reviewer recommended that an industrial partner—beyond “dissemination of data”—would be desirable.

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 remarked that the directions of future research are appropriate, and time will tell if any of the directions will be fruitful.

Reviewer 2:

The reviewer commented that the future direction seems to be lithium nickel manganese cobalt aluminum oxide (NMCA), which is reasonable. It will be interesting to see the progress in the later years, especially how to achieve both thermal stability and high energy density.

Reviewer 3:

The reviewer noted that there are several outstanding issues with these cathode materials, i.e., poor thermal stability, increased metal dissolution and capacity fade, and higher reactivity towards electrolytes with the Ni-rich formulations. In addition to the providing higher specific capacity, these cathodes need to function well at higher loadings. The reviewer said that, appropriately, the future studies will address these issues, and these studies are consistent with DOE goals of high specific energy, low-cost, and safe Li-ion batteries.

Reviewer 4:

The reviewer said that the proposed future research aimed at energy and durability improvement is quite comprehensive and if successfully completed will contribute significantly to the Battery 500 goals. The reviewer recommended showing the Wh/l values of the cells so that reviewers can have an appreciation of the cell system in question.

Reviewer 5:

The reviewer said that as was discussed during the review meeting, there may be a different set of challenges as the team moves from 300 Wh/kg to the final goal of 500 Wh/kg using Ni-rich NMCs/Li-metal. The reviewer recommended that it would be helpful to identify what these challenges are early in the project (not just the challenges encountered in achieving 300 Wh/kg) to guide the project. The reviewer was unclear from the presentation whether the team has multiple approaches and options to tackle the problems identified: minimizing cracking and mechanical degradation, and improving ionic and electronic conductivities.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer pointed out that a higher capacity cathode is a key requirement for developing a cost-effective, safe and high-energy battery to support DOE's overall goal. This project is thus extremely relevant.

Reviewer 2:

The reviewer said that for a widespread use of EVs, the batteries need to be lightweight, compact, safe, and of low-cost. The state-of-the-art Li-ion batteries are inadequate to fulfil these needs. Higher energy density and lower cost cathode materials are required to improve the specific energy for Li-ion cells and reduce overall cost for the battery. The reviewer said that state-of-the-art cathode materials provide capacities of only ~170 mAh/g, which needs to be increased to greater than 220 mAh/g to achieve the cell level energy of 500 Wh/kg. Battery researchers need to develop new Ni-rich cathode materials, which the present project is duly addressing.

Reviewer 3:

The reviewer said yes, and clarified that a high-energy density cathode is one of the key issues to achieve overall energy density of the battery.

Reviewer 4:

The reviewer said that the project supports the overall DOE Battery 500 objectives.

Reviewer 5:

The reviewer observed good relevance.

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

Reviewer 1:

The reviewer said that the team has sufficient resources for the project with one possible exception in the area of measuring and understanding mechanical behavior and degradation of Ni-rich NMC electrodes.

Reviewer 2:

The reviewer found that the total funds should be sufficient for the project team members to complete the tasks on schedule.

Reviewer 3:

The reviewer said that resources are okay.

Reviewer 4:

The reviewer said that resources are sufficient to carry the work.

Reviewer 5:

The reviewer said that the resources are adequate for the scope of the project, though the reviewer was not clear what the specific budget for BU is (and individual organizations in the Battery 500).

Presentation Number: bat360
Presentation Title: Overview and Synthesis of High-Nickel Nickel Manganese Cobalt Oxide (NMC) Cathodes
Principal Investigator: Arumugam Manthiram (University of Texas-Austin)

Presenter

Arumugam Manthiram, University of Texas-Austin

Reviewer Sample Size

A total of five reviewers evaluated this project.

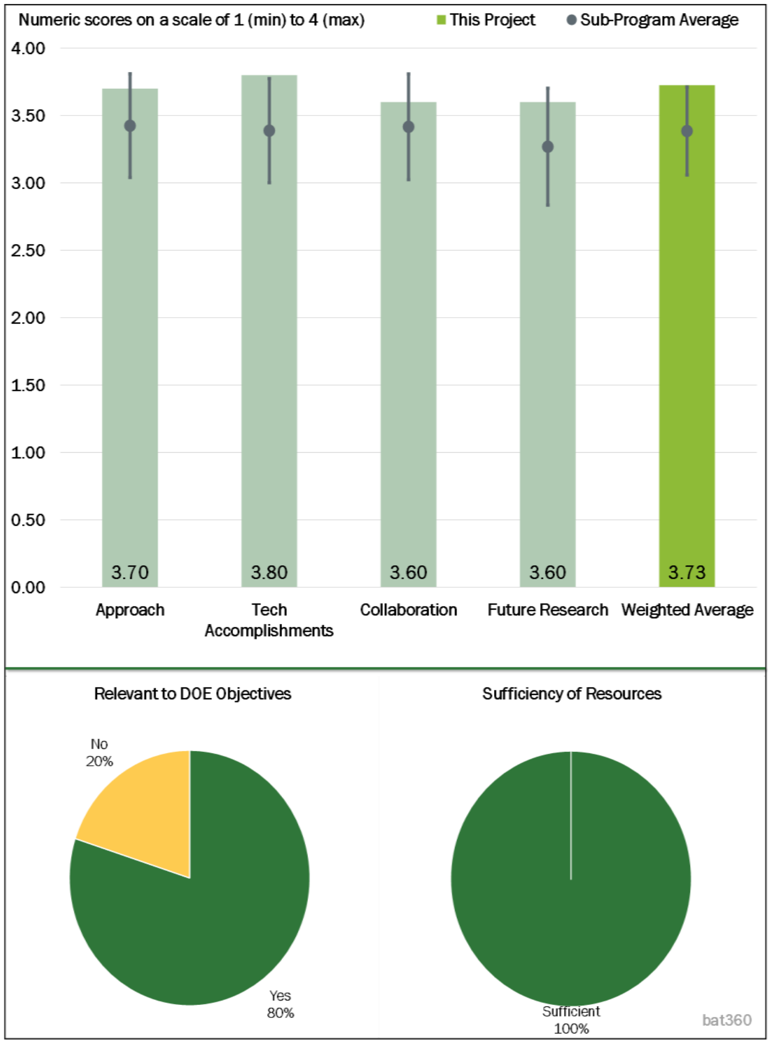

Figure 2-61 - Presentation Number: bat360 Presentation Title: Overview and Synthesis of High-Nickel Nickel Manganese Cobalt Oxide (NMC) Cathodes Principal Investigator: Arumugam Manthiram (University of Texas-Austin)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer noted that the key barrier to achieving the Battery 500 objective is directly addressed in this project by focusing on the main bottleneck, i.e., the cathode. The team is directing its efforts to further enhancing the properties of currently used and already mature layered cathodes in order to increase the capacity without comprising durability, safety, and cost. The reviewer remarked that the project is highly focused with a well-organized research plan.

Reviewer 2:

The reviewer observed clearly stated objectives and stressed that discussion of how the team will try to reach them was also included.

Reviewer 3:

The reviewer said that the project approach, i.e., small percentage elemental doping to address the stability issue, is good.

Reviewer 4:

The reviewer asked what the goal of scaling up synthesis for the project is. The target of 500 g or 1,500 g per batch seems quite arbitrary, especially because it appears to be all based on trial-and-error instead of a process model.

Reviewer 5:

The reviewer said that the project is well-designed and feasible. The reviewer commented that although the secondly particle size is well-controlled and uniform for all nickel cobalt manganese oxide (NCM), the PI may want to investigate the correlation between Ni content and the morphology of the primary particle. The reviewer said that the primary particle will influence the electrochemical performance, degradation, and air stability.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that high-Ni NMC characterizations are underway, which is good. Using Al doping to suppress air-sensitivity and improve cyclability has been shown, which the reviewer characterized as really impressive for this early in the project. The reviewer said that scale-up is excellent, with great early results.

Reviewer 2:

The reviewer said that within a short time, less than 2 years, the technical accomplishment is excellent.

Reviewer 3:

The reviewer said that the PI focused on the major technical barriers and made significant progress.

Reviewer 4:

The reviewer remarked that the project has made significant progress towards understanding the structure-stability-capacity relationships of the layered cathodes with a view to improving their capacity. The team was able to produce both 811 and 900505 cathode materials in large batches that demonstrated better performance than commercial materials (622 and 811). (The reviewer cautioned that not all commercial samples represent the state of the-art and hence drawing absolute conclusions can be risky unless well-known suppliers are benchmarked). The reviewer said that work related to air-sensitivity is quite comprehensive. The authors carried out an insightful work on the effect of Al-doping in 9406 material that showed how it reduces lattice strain. The reviewer pointed out that most of the slides are also very self-contained with a nice take-home message at the end of the slides.

Reviewer 5:

The reviewer said that air and moisture sensitivity and stability of the NMCs should be quantitatively defined. The reviewer noted that the commercial NMC811 by TODA America (see the BAT164 presentation) seems to be stable in water, and asked why. The reviewer asked what mechanisms are responsible for the secondary particle pulverization. The team should collaborate with people who can measure the mechanical properties and fracture strength of particles.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the project has excellent collaboration among the team-members.

Reviewer 2:

The reviewer pointed out that the PI actively collaborates with other teams within Battery 500.

Reviewer 3:

The reviewer said that the collaboration among team members is excellent.

Reviewer 4:

The reviewer remarked that the collaboration within the Battery 500 team seems strong. However, the team may benefit from collaborations with other DOE funded project teams, especially because many have or are working on Ni-rich NMCs.

Reviewer 5:

The reviewer said that the project would benefit from industrial collaboration

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

Reviewer 1:

The reviewer found that future directions are very well-defined, much better than in most other projects; and in the right directions.

Reviewer 2:

The reviewer remarked that the future work, i.e., optimizing cathode synthesis, and surface/bulk stabilization, are important to achieve high energy density and stability oxide cathodes.

Reviewer 3:

The reviewer said that the proposed future research goals emphasizing higher capacity, durability, and safety are critical. Although not explicitly highlighted, the reviewer expressed certainty that the team will be focusing on reducing the Co content to as low as possible in order to lower cost.

Reviewer 4:

The reviewer remarked that as was discussed during the review meeting, there may be a different set of challenges as the team move from 300 Wh/kg to the final goal of 500 Wh/kg using Ni-rich NMCs/Li-metal. The reviewer thought that it would be helpful to identify what these challenges are early in the project (not just the challenges encountered in achieving 300 Wh/kg) to guide the project.

Reviewer 5:

The reviewer said that the PI plans to explore the long-term cyclability of NMC811 with various charge voltage cutoffs (4.2V-4.5V). If charging Ni-rich to higher voltage beyond 4.4V, the PI should have a thorough energy density/cycling stability comparison of Ni-rich oxides with high Mn or high-Co NCM.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said yes, and elaborated that the PI is trying to achieve Battery 500 objectives.

Reviewer 2:

The reviewer remarked that a high energy density oxide cathode is one of two approaches to achieve the overall goal of the Battery 500 program.

Reviewer 3:

The reviewer said that development of a high-capacity cathode that meets other battery requirements such as safety, durability, and cost will support DOE's objective of a high-energy density battery.

Reviewer 4:

The reviewer said that the project supports the overall DOE Battery 500 objectives.

Reviewer 5:

The reviewer said high energy density.

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 team has sufficient resources for the project, with one possible exception in the area of measuring and understanding mechanical behavior and degradation of Ni-rich NMC electrodes.

Reviewer 2:

The reviewer said that the resources are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 3:

The reviewer said that the resources should be sufficient to achieve the milestones of the project on schedule.

Reviewer 4:

The reviewer said that resources are okay.

Reviewer 5:

The reviewer indicated that resources are sufficient to carry out the work.

Presentation Number: bat361
Presentation Title: Lithium-Sulfur Batteries: From Materials Understanding to Device Integration
Principal Investigator: Yi Cui (Stanford University)

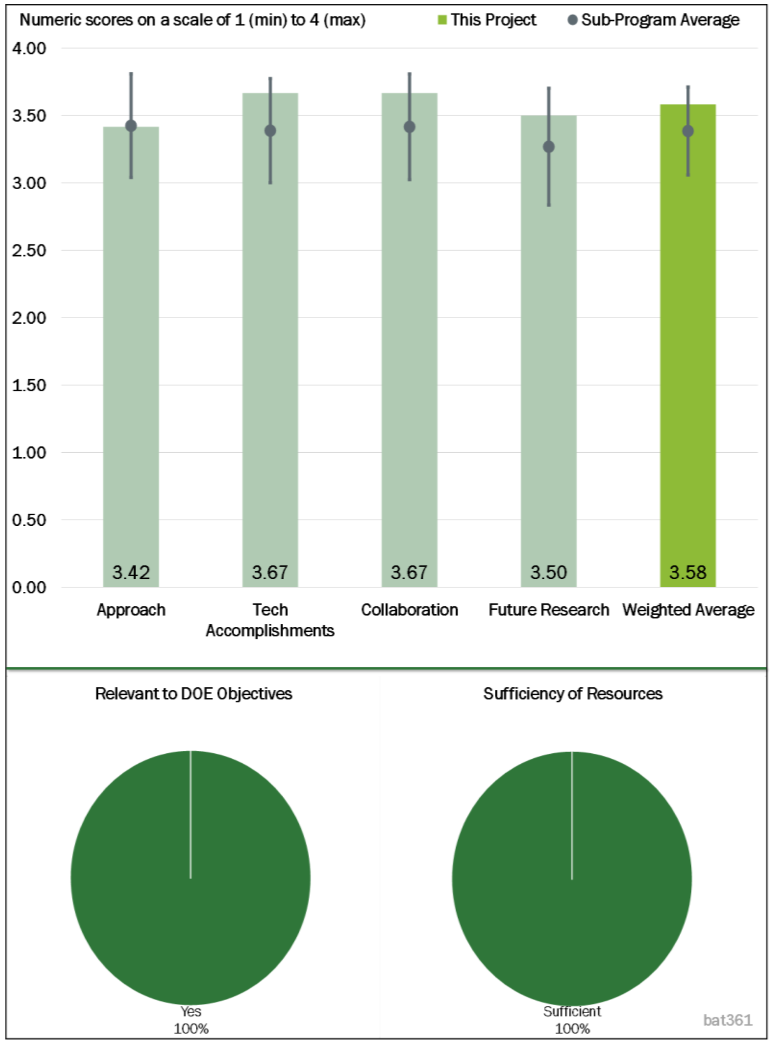

Figure 2-62 - Presentation Number: bat361 Presentation Title: Lithium-Sulfur Batteries: From Materials Understanding to Device Integration Principal Investigator: Yi Cui (Stanford University)

Presenter

Yi Cui, Stanford University

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 and well-planned.

Reviewer 1:

The reviewer remarked that the Stanford/PNNL team has done excellent in developing high-energy Li-S batteries (high capacity and stability with long cycle life) through materials understanding and selection and device Integration, with the goal of achieving 500 Wh/kg specific energy to power EVs at low cost. The team has completed the baseline properties of the Li-S cathode required to reach 300 Wh/kg based on Battery 500 cell design. Developing polymer membranes and Li-metal protection methods is of great interest. The reviewer found that the project has made remarkable progresses in addressing the technical barriers.

Reviewer 2:

The reviewer said that the approach taken by the team that leverages its expertise in nanomaterial design and synthesis combined with novel assembly and simulations to develop the Li-S battery clearly addresses the key technical barriers to achieve the objectives of the Battery 500 program.

Reviewer 3:

The reviewer remarked that the S nanostructure and Li-metal anode modification approaches are well designed and feasible. The S catalyst works, is new, and needs more research attention.

Reviewer 4:

The reviewer said that energy/volume, in addition to energy/mass, should be considered if the Li-S research is aimed at automotive applications.

Reviewer 5:

The reviewer observed that the presentation identified many approaches. The reviewer expressed confusion about which one or few is/are specifically with this project.

Reviewer 6:

The reviewer pointed out there was no mention of volumetric energy density, which is of primary importance for vehicles.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented brilliant and extremely innovative work on addressing S battery limitations. The reviewer was especially impressed with the very novel work on enabling Li-metal

Reviewer 2:

The reviewer said that the team has demonstrated several significant technical accomplishments and progress towards the overall project. The project is in good shape in terms of milestones.

Reviewer 3:

The reviewer found that lots of excellent progress has been demonstrated.

Reviewer 4:

The reviewer said that it is very helpful to standardize Testing Requirements and Protocols for Li-S cells.

Reviewer 5:

The reviewer commented that thanks to a multitude of innovative concepts and studies, the team has achieved a number of significant results that demonstrate measurable progress towards the program goals. This is evidenced, among others, by the number of publications in high-quality journals. The reviewer said that the team deserves kudos for their novel work. Despite this progress, the fundamental issues both at the Li as well as the S electrodes remain. The reviewer was unclear how these approaches affect the energy density of the cell (Wh/l) because the reviewer did not find in the presentation the actual composition of the S electrode. It will be useful to report this metric in future presentations for ease of understanding. The reviewer said that among the Li hosts, SiO and aluminum fluoride (AlF_3) look interesting but again it is unclear how the Wh/l values get affected by the hosts and how to tailor the amount of Li desired.

Reviewer 6:

The reviewer said that the statement in one of the slides under Accomplishment, “Pouch cell: Multilayer stacking/pressing and lean electrolyte brings more challenges than in Li/NMC cells,” does not convey much information. The reviewer inquired what the challenges are, and how the team is going to solve these challenges.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the project has a strong collaboration across the team members. This is evidenced by the fascinating work involving cryogenic electron microscopy that allowed resolution down to individual Li atoms.

Reviewer 2:

The reviewer found that the collaboration within the Battery 500 team seems strong.

Reviewer 3:

The reviewer said that the team has been collaborating with faculty at Stanford University and the University of California-Los Angeles (UCLA). The collaboration is very productive.

Reviewer 4:

The reviewer pointed out that the PI actively collaborates with other teams within Battery 500.

Reviewer 5:

The reviewer said that the collaborations between this project and other team members are clearly demonstrated during the presentation.

Reviewer 6:

The reviewer recommended that the project would benefit from industrial participation.

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

Reviewer 1:

The reviewer stated that this project has the best chance of solving the Li-metal problems.

Reviewer 2:

The reviewer found that the proposed future work is well-planned. The team will focus on several key tasks, such as the interaction between S species and multifunctional binders, and select the optimal materials to re-capture the active S species diffused in the electrolyte. The reviewer detailed that the plan to test S cathodes with high areal mass loading at high current densities may lead to new findings. Developing 3-D Li-metal anodes and stable electrolytes holds a great promise.

Reviewer 3:

The reviewer described proposed future work as obvious and to-the-point—how to improve durability at an acceptably high cathode loading. This has been a formidable challenge for decades now and hopefully the novel approaches proposed might bring about significant improvement to the results. The reviewer referenced the use of solid electrolytes, and inquired if it is a part of the Battery 500 program.

Reviewer 4:

The reviewer noted that energy/volume should be a key consideration of a go/no-go decision if the Li-S research is to go forward for EV applications.

Reviewer 5:

The reviewer said that besides the proposed future research, the PI may want to improve the rate capability by understanding catalyst effect on S reaction kinetics.

Reviewer 6:

The reviewer found that many promising concepts and progress have been demonstrated. The reviewer said that it will be great if the future research can be a little bit more focused.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer commented that the development of a high-capacity S cathode and a stable Li anode is the key task of the Battery 500 program that directly supports the DOE objectives of a low-cost, high-energy density battery,

Reviewer 2:

The reviewer said that energy/volume should be key considerations of a go/no-go decision if the Li-S research is to go forward for EV applications.

Reviewer 3:

The reviewer stated that the team has been working on the design and fabrication of S cathodes with high capacity and stability with long cycle life, and Li-metal anodes with high capacity, high CE, and long cycle life, which is critical for commercialization of Li-S batteries and highly relevant to VTO program goals.

Reviewer 4:

The reviewer remarked that the alkali metal-S chemistry should always be one of the research focus areas towards high-energy density batteries. Further, this reviewer asserted that the project supports Battery 500 objectives.

Reviewer 5:

The reviewer said that the project clearly addresses one of two approaches (S and layered-oxide) in developing a high-energy cathode.

Reviewer 6:

The reviewer remarked high energy density.

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 given the quality and quantity of results that come out of Professor Cui's lab, the resources seem insufficient and should be increased, unless his team is provided additional funding via other routes. The reviewer was unsure about interpreting the funding level listed on the presentation.

Reviewer 2:

The reviewer said that the team has sufficient resources for the project.

Reviewer 3:

The reviewer remarked that the team has fully used the resources at Stanford, PNNL, and UCLA through collaboration.

Reviewer 4:

The reviewer said that resources are sufficient.

Reviewer 5:

The reviewer remarked that resources for the project are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 6:

The reviewer said resources are okay.

Presentation Number: bat362
Presentation Title: Lithium-Metal Anodes: Problems and Multiple Solutions Based on Hosts, Interphase, and Electrolytes
Principal Investigator: Jun Liu (Pacific Northwest National Laboratory)

Presenter
Jun Liu, Pacific Northwest National Laboratory

Reviewer Sample Size
A total of five reviewers evaluated this project.

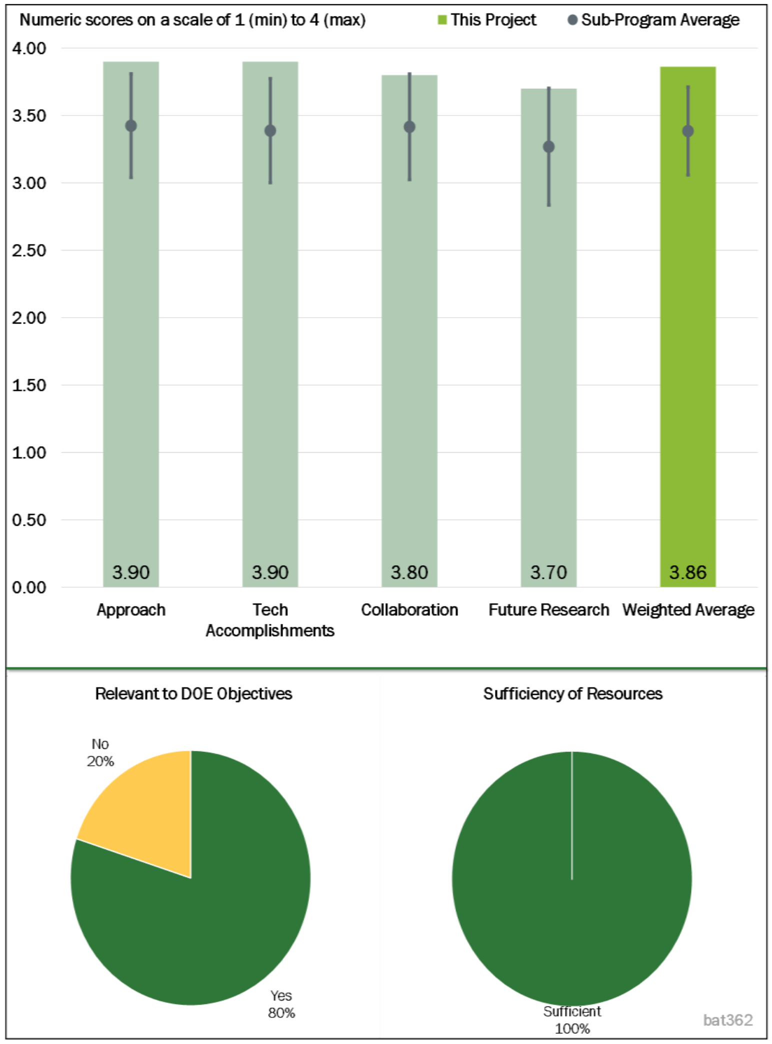

Figure 2-63 - Presentation Number: bat362 Presentation Title: Lithium-Metal Anodes: Problems and Multiple Solutions Based on Hosts, Interphase, and Electrolytes Principal Investigator: Jun Liu (Pacific Northwest National Laboratory)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:
The reviewer said that the team has put in place a very comprehensive approach sharply focused on resolving the issues that plague Li anode cyclability. It is the best concerted effort the reviewer had ever seen to tackle this decades-old Li anode problem. This is a very carefully thought-out and planned project that is also implementable.

Reviewer 2:
The reviewer remarked that a localized high-concentration electrolyte (LHCE) approach is very well-designed. It retains all advantages of high-concentration electrolyte at a low cost. The reviewer praised that this is one of the best electrolyte works this reviewer has seen over recent years.

Reviewer 3:
The reviewer remarked that the team is attacking with three very good approaches—more stable electrolytes, improved protection layers, and new hosts. The team is also developing new methods to detect Li-metal.

Reviewer 4:
The reviewer said that the approach is highly comprehensive, including modeling and experiments in stable electrolytes, hosts for Li and S, protective layers, and detailed characterization.

Reviewer 5:
The reviewer said that the electrolyte additive and optimization are very important to achieving the stability of a Li-metal anode.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that significant progress seems to have been made towards improving the cyclability of the Li anode. Just to see cycle-life data up to 700 or so at reasonably high current density of 2 mA/cm^2 or so is quite refreshing and encouraging (please do show the data until the end so that people have a good idea about the failure mode). The reviewer said that it is very interesting to see how concepts like LHCE are significantly improving Li anode cyclability. The reviewer pointed out that quite a few novel ideas from the consortium labs are being explored, and the reviewer hopes that one of these ideas or a combination thereof will allow for the development of a practically useful Li cell.

Reviewer 2:

The reviewer observed a very sophisticated and innovative work to find an acceptable electrolyte with a high concentration, taking advantage of a deep understanding of ion transport. The reviewer is very impressed with how the team has combined theory and experiment to develop the improved electrolyte. The reviewer noted that experimental results are impressive, especially given that the experiments are not requiring high-cost surface engineering or high-cost additional steps in cell fabrication.

Reviewer 3:

The reviewer observed excellent progress demonstrated within a little more than one year.

Reviewer 4:

The reviewer said that the PI achieved the milestones and the progress is excellent.

Reviewer 5:

The reviewer remarked that accomplishments are numerous and impressive. The statement on one of the slides that the silly putty is “solid-like upon stress” is inaccurate. The reviewer said that it is solid-like under a high strain-rate.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found that the collaboration within the Battery 500 team seems strong.

Reviewer 2:

The reviewer noted an outstanding collaborative team that brings together scientists having complementary strengths is carrying out this project.

Reviewer 3:

The reviewer said that collaboration with other members of the team has been clearly demonstrated.

Reviewer 4:

The reviewer said that the PI actively collaborates with other teams within Battery 500.

Reviewer 5:

The reviewer said that the project would benefit from industrial collaboration.

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

Reviewer 1:
The reviewer found that future work plans are clearly identified. This project will focus on developing 3-D host for Li-metal, and electrolyte additives. The reviewer pointed out that both are important for the Li-metal anode development.

Reviewer 2:
The reviewer said that the team is attacking the proper challenges.

Reviewer 3:
The reviewer observed that the team has proposed an exhaustive list of future work directed at improving the CE of the Li anode using the electrolyte concept, host structures, etc. These seem quite reasonable. The reviewer said that, however, the team should leverage lessons learned from other work as much possible to come up with a practically useful solution for this difficult problem. Working with systems that can be prohibitively expensive or difficult to manufacture or have not shown a robust solution should not be pursued for the sake of research alone. In this regard, the reviewer thought of very concentrated salt systems (cost), polymer coating (do they really work?), and vapor phase treatment of Li surface (manufacturability) among others.

Reviewer 4:
The reviewer commented that the desired attributes for protective layers for Li-metal electrodes should be identified and quantified to enable the project to go forward.

Reviewer 5:
The reviewer remarked that the PI may focus more on the fundamental understanding and optimization of LHCE and investigate the LHCE stability on the cathode side, especially when charging to higher voltage beyond 4.4V.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that this project supports the overall Battery 500 objective very well. It demonstrates an innovative approach to stabilize Li-metal, which is the key to achieving high energy density.

Reviewer 2:
The reviewer said that the Li-metal anode is the major issue to reach the energy density goal for the program.

Reviewer 3:
The reviewer pointed out that development of a well-functioning Li anode will be a major breakthrough towards the goal of the 500 Wh/kg cell that will directly support DOE’s overall objectives.

Reviewer 4:
The reviewer found that the project supports the overall DOE Battery 500 objectives.

Reviewer 5:
The reviewer said energy density.

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

Reviewer 1:
The reviewer found that the team has sufficient resources for the project.

Reviewer 2:
The reviewer said that the resources allocated should be sufficient to complete the tasks on schedule

Reviewer 3:
The reviewer said that resources for the project are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 4:
The reviewer observed sufficient resources to carry out the proposed work.

Reviewer 5:
The reviewer said that resources are okay.

Presentation Number: bat363
Presentation Title: Understanding Performance Limitations in Thick Electrodes, Ping Liu
Principal Investigator: Ping Liu (University of California-San Diego)

Presenter

Ping Liu, University of California-San Diego

Reviewer Sample Size

A total of five reviewers evaluated this project.

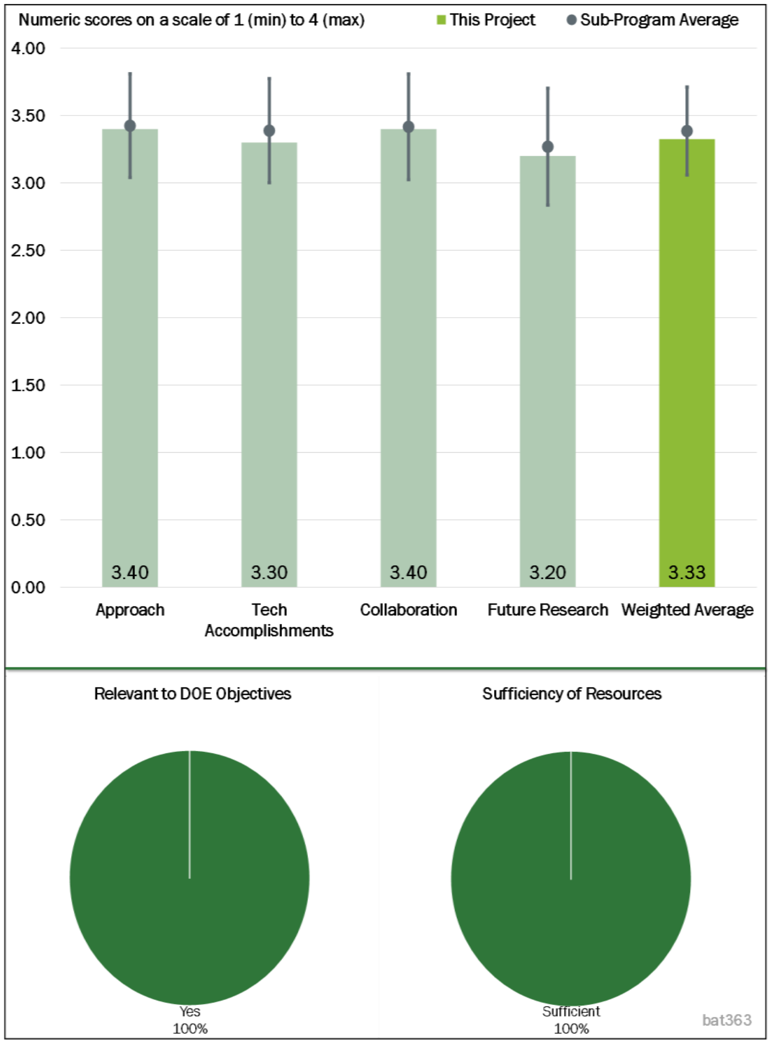

Figure 2-64 - Presentation Number: bat363 Presentation Title: Understanding Performance Limitations in Thick Electrodes, Ping Liu Principal Investigator: Ping Liu (University of California-San Diego)

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The reviewer said that the project is focused on the development of high loading cathodes by addressing factors that limit the performance of such electrodes. Effect of binders, use of open channels to enhance conductivity, as well as studies to delineate electronic and ionic conductivities are important aspects, among others, that need to understood to develop well-functioning thick electrodes

Reviewer 2:

The reviewer detailed that the goal of the overall Battery 500 project is to achieve a cell level specific energy of 500 Wh/kg through using high-capacity cathodes consisting of Ni-rich NMC or a S cathode, Li anode, and compatible electrolyte. High-capacity, Ni-rich NMC cathodes are being investigated by a few PIs in this project. However, a more likely solution, at least in the near-term, would be to develop thick electrodes to reduce amount of inactive materials to achieve proportionate gains in the specific energy. The reviewer said that analysis shows that this approach will also have a benefit in cost, because of the reduced quantities of separator, electrode substrates, etc. The challenge, however, is to ensure that the cathode is fully utilized through its depth, which requires cathode designs with low tortuosity, adequate electrolyte penetration etc., which this project is addressing. The reviewer found that this project is well designed and integrated with the goals and the other efforts under Battery 500.

The only difficulty with this approach is that several commercial (18650 cell) manufacturers have already achieved improved specific energies (greater than 50 wh/kg) with a dense cathode from state-of-the-art materials, and it is not clear if there is room for further improvements in this direction. The reviewer found that nevertheless, it is good that additional performance-governing paraments (ionic and electronic conductivity) are being evaluated with a dense cathode form industrial partners.

Reviewer 3:

The reviewer detailed that the project is trying to understand the thick electrode performance, and establish performance baseline for the 622 and 811 electrodes from various vendors.

Reviewer 4:

The reviewer said that the approach encompasses important goals, but it is quite vague. The reviewer asked how these goals are going to be attacked. This is more about characterizing, rather than optimization.

Reviewer 5:

The reviewer said that the project may need to identify more thick-electrode design parameters and study the effect of these design parameters (e.g., packing density, particle size distribution within electrode) on the electrochemical performance.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer commented that the PI achieved the milestones and the progress is excellent.

Reviewer 2:

The reviewer remarked the team obtained quite a few interesting results that are helpful for designing thick electrodes. The coherent X-ray diffraction imaging (CXDI) results are worth noting along with work on the separation of electronic and ionic resistances of thick electrodes. The reviewer said that the 811 cathode image is impressive. The reviewer asked if the experiments can be done at higher temperatures to accelerate the degradation.

Reviewer 3:

The reviewer said that during the first year of the project, there seems to be two major accomplishments/findings: finding inhomogeneity in thick electrodes; and identifying the pros and cons of a “crack” approach.

Reviewer 4:

The reviewer found that good progress has been made on the NMC-622 and -811 cathodes in understanding the effect of loading on performance, in demonstrating good performance with dense (30 mg/cm^2) cathodes, and in verifying that these cathodes have structural stability but undergo structural reconstruction during cycling. Interestingly (but not unexpectedly) the poor utilization of the active material in a dense cathode has been verified from in operando CXDI imaging. However, whether it helps this in the design of thick cathodes was unclear to this reviewer, who asked whether it can be as quantify of electrochemical data. Ionic conductivity has been improved in dense cathodes (120 microns) by mud-cracking, but the electronic (contact) resistance has been found to increase. The reviewer said that it may be challenge to lower the ionic and electronic resistances simultaneously. The reviewer suggested doing the cathode design optimization with NMC 811 directly, instead of 622 (to avoid design modifications later on), provided suitable 811 or 900505 and with suitable particle size is available. Overall, this reviewer observed good progress in the first year of this project.

Again, based on this reviewer’s understanding, industry has achieved cathode a loading higher than 30mg/cm^2, though with NCA. The reviewer commented that it may be worthwhile to collaborate with a battery manufacturer, if possible. Also, DOE funded some projects in the past on developing thick cathodes. The reviewer asked if there is there anything to learn from them, especially 24M’s prior efforts.

Reviewer 5:

The reviewer said the team identified that binder is important, and that 811 structure is very robust. The reviewer was a little dubious about interpreting the inhomogeneity measurements. They seem pretty crude at this point, but maybe the team can do better in the future. By only looking at a very small number of particles, the reviewer was unsure that the statistical power of the measurements is significant. BNL seems to have a much more quantitative approach. The importance of electronic resistance was demonstrated.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said that the team has excellent collaboration across the team members.

Reviewer 2:
The reviewer commented that there are very good collaboration activities with the PIs in the Battery 500 projects, with researchers from PNNL, UCSD, UT-Austin, and BU. The reviewer suggested more active collaboration with industrial battery manufactures and also with the national laboratories DOE previously funded for similar efforts.

Li, Zheng

The reviewer suggested that the PI can collaborate more with the materials synthesis team to study how the materials properties will impact the overall thick electrode performance.

Reviewer 3:
The reviewer commented that the samples seem to be provided by industrial partners.

Reviewer 4:
The reviewer said that the project would benefit from industrial collaboration.

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

Reviewer 1:
The reviewer said that there are several outstanding issues with the dense cathode designs to reduce tortuosity without raising electronic resistance and to demonstrate long-term cycling stability in proper cells, without being limited by the Li anode, all of which will be addressed in the proposed future studies. These studies are consistent with DOE’s goals of high specific energy, low-cost, and safe Li-ion batteries.

Reviewer 2:
The reviewer said that the three approaches proposed in the “future work” section are important.

Reviewer 3:
The reviewer remarked that the proposed future research (electrode homogeneity, conductivity enhancement, etc.) look okay but the reviewer is unsure one can achieve the loading level that is the target of the Battery 500 program.

Reviewer 4:
The reviewer found that future projects are rather vague, although they are pointing in the right direction.

Reviewer 5:
The reviewer pointed out that Battery 500 proposed two chemistries. The future research should include work on designing S thick electrode and understanding the performance limitations.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer detailed that for a widespread use of EVs, the batteries need to be lightweight, compact, safe, and of low-cost. The state-of-the-art Li-ion batteries are inadequate to fulfil these needs. Higher energy density and lower-cost cathode materials are required to improve the specific energy for Li-ion cells and reduce overall cost for the battery. The reviewer said that the state-of-the-art cathode materials provide capacities of only ~170 mAh/g, which needs to be increased to greater than 220 mAh/g. Also, the cathode loading will have to increase by ~25% to achieve the cell level energy of 500 Wh/kg. The reviewer said that proper cathode designs are to be developed that will enhance ionic conductivity without impairing electronic counterpart, with the emerging cathode materials, which the present project is duly addressing.

Reviewer 2:
The reviewer commented that a thick electrode is essential to achieving high battery energy density, and that this project supports the Battery 500 objectives.

Reviewer 3:
The reviewer agreed that high cathode loading is definitely necessary to achieve the final program goal.

Reviewer 4:
The reviewer said that using thick electrodes minimizes cell cost and so this project has direct relevance to DOE's objective of a low-cost battery.

Reviewer 5:
The reviewer said high energy density.

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 the resources should be sufficient for the team to complete the tasks on schedule.

Reviewer 2:
The reviewer commented that the resources for the project are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 3:
The reviewer said that resources seem to be sufficient to carry out the proposed research.

Reviewer 4:
The reviewer said resources are okay.

Reviewer 5:
The reviewer commented that the resources are adequate for the scope of the project, though it is not clear what the specific budget is for this group at UCSD (and individual organization in Battery 500).

Presentation Number: bat364
Presentation Title: Coatings for Cathode and Separator
Principal Investigator: Jihui Yang (University of Washington)

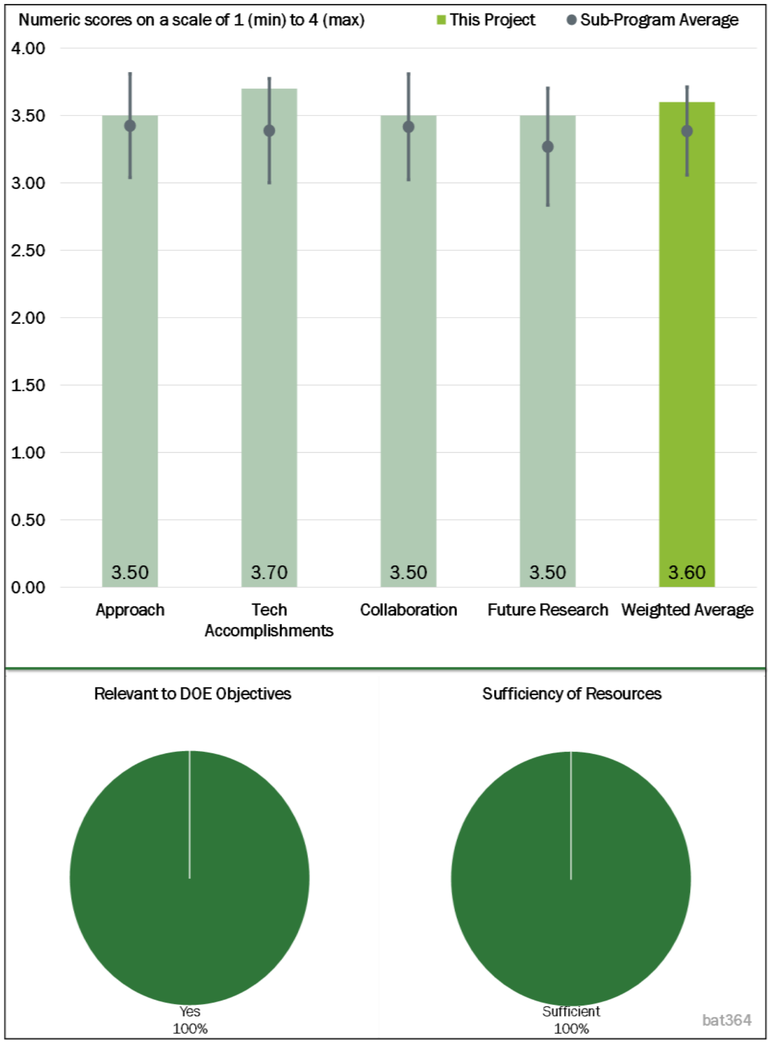

Figure 2-65 - Presentation Number: bat364 Presentation Title: Coatings for Cathode and Separator Principal Investigator: Jihui Yang (University of Washington)

Presenter

Jihui Yang, University of Washington

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 and well-planned.

Reviewer 1:

The reviewer remarked that surface stability has been shown as one critical issue for the practical use of Ni-rich NMC cathodes in batteries. Surface coating via ALD appears to be an outstanding approach for protecting Ni-rich NMC cathodes from direct contact with the electrolyte and thereby improving the cycling stability. The reviewer said that the technical feasibility has been well demonstrated in this project, through extensive electrochemical tests and characterization using multiple techniques.

Reviewer 2:

The reviewer remarked that the approach is in-line with the Battery 500 technical challenges. The PI aims to tackle the interfacial problems of the NMC cathode and state-of-the-art separators with surface modification, and to combine the cathode and separators with a Li-metal anode. The reviewer remarked that the approach is appropriate and effective to improve the conductivity and uniformity of Li deposition, both of which are considered as the major technical obstacles for Battery 500.

Reviewer 3:

The reviewer commented that the team has done an excellent in studying the coatings for cathodes and separators in Li-ion batteries. The team has developed a mixed conductor surface coating for Ni-rich NMC materials to improve their interfacial and cycling stability. The reviewer pointed out the team has also identified a separator coating to improve the CE and cycling stability of a Li-metal anode. The project started in 2017 and has made remarkable progresses in addressing the technical barriers.

Reviewer 4:

The reviewer said that the approach with respect to synthesis and reactivity is good. The main technical barriers (particularly in the coated separators) will be centered around the mechanical properties. The reviewer thought that perhaps more understanding of ceramic coated separators versus ceramic impregnated separators would be helpful.

Reviewer 5:

The reviewer summarized that the approach involves ALD coating on NCM cathodes in combination with solid electrolyte coatings on Li-metal to achieve high-energy density cells. The reviewer thought that while it is interesting and worth to be explored, it is unclear how this approach is different than similar approaches explored in other academic studies, why coating the separator may overcome the current limitations of the solid electrolyte coatings on Li foils (nearly all of which suffer from failures at grain boundaries), and if ALD coating is economical and fundamentally better than gradient commercial cathodes with solution-deposited layers.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that the PI has made significant accomplishments in all three areas listed in the Technical Approach. The team tried different Al surface coatings and found that AlF_3 improved the cycle life of 811 NMC, which is the target cathode material for Battery 500; the separator coated with Li-ion conductive material can up-take more liquid electrolyte and establish an “artificial” SEI layer on a Li anode and therefore, reduce the dendrite growth on the Li anode. The reviewer said that the performance of the whole cell was improved.

Reviewer 2:

The reviewer said that the project milestones have been completed according to project plan and appear to be on track for next goals.

Reviewer 3:

The reviewer remarked that all of the milestones have been completed. Significant progress has been made in improving the interfacial and cycling stability of NMC811 by ALD coating. The reviewer commented that achieving 80% capacity retention for 300 cycles is outstanding. In addition, good progress has also made in ALD coating on separators.

Reviewer 4:

The reviewer remarked that the team has demonstrated several technical accomplishments and progresses toward overall project. The project is in good shape in terms of milestones. The reviewer suggested that tensile and penetration/puncture tests be carried out on the coated separators.

Reviewer 5:

The reviewer noted that the authors demonstrated in situ XRD to measure structural stability of 811; identified that the initially proposed sol-gel $LiAlO_2$ is not very effective (very high sensitivity to moisture; forming inert hydroxide and carbonates on the surface leading to high impedance); observed that ALD of AlF_3 on 811 particles (5-10 nm) improve cycling stability in half cells; and observed that thin coating (“30AlF^3) does not change diffusivity and rate performance, while thicker “60AlF_3” ALD coating does affect rate performance (in thick electrodes 7 mg/cm2). The authors observed that “regular”/”uncoated” NMC811 suffers from particle corrosion and metal dissolution. Finally, the authors found that LLZO and 5-10 wt. % polyethylene oxide with LLZO particles (15 microns in thickness) on the surface of a commercial Celgard separator show better performance than uncoated separators (although not nearly at the levels acceptable for use). The reviewer pointed out that many commercial 811 now show significantly better performance than what was demonstrated (which might be expected because industry invests in similar projects as well). Overall, the reviewer thought it would be beneficial if the authors would focus more on fundamentals and use ALD to tune coating chemistry systematically.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer observed a wide collaboration within the Battery 500 Consortium and externally (with GM), on materials synthesis/characterization and ALD coating, has been well demonstrated. One good example is the joint publications from the collaborations.

Reviewer 2:

The reviewer said that the PI intensively collaborated with PIs within Battery 500 and with an industry partner too.

Reviewer 3:

The reviewer remarked that the degree of collaboration is inherent in the Battery 500 consortium. It is a multi-pronged effort from many groups

Reviewer 4:

The reviewer commented that the authors collaborated with PNNL on separator coating and solid electrolyte modification, with GM on ALD coating of Ni-rich NMCs, and with UT-Austin and BU on Ni-rich NMC synthesis and characterization, including in situ XRD.

Reviewer 5:

The reviewer said that the PI has demonstrated several good collaborations with PNNL, GM, UT-Austin, and BU. The reviewer suggested that the PI reach out to collaborate with modeling groups to design the coatings.

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

Reviewer 1:

The reviewer noted that this is the middle of the second-year report. The PI presented a clear plan leading to the accomplishment of the on-going efforts of coating NMC811 cathode with AlF_3 and other materials, further optimization of separator coating. The reviewer said that the future work is based on the solid achievement of the project so far.

Reviewer 2:

The reviewer said that the proposed future work is well-planned. The reviewer suggested that the team study the bonding between the coating and the cathode/separator during/after cycling.

Reviewer 3:

The reviewer said that future research has been well-planned, on in-depth characterization of the surface ALD coating, and developing new coating materials/techniques. The reviewer said that more efforts are needed for integrating the ALD coating both on cathodes and on separators.

Reviewer 4:

The reviewer found that the proposed future research for cathode coating is reasonable based on results. The project is proposing to look at the mechanical properties of the separator coating. According to the reviewer, one area that is not mentioned is the adhesion of the coating to the separator, which could be a problem based on the mismatch of expansion properties of the ceramic versus the polymer.

Reviewer 5:

The reviewer detailed how the authors proposed to study three types of ALD coating on NMC811 (aluminum phosphate; $Li_{1+x}Al_xTi_{2-x}(PO_4)_3$ [LATP], and Li_3NbO_4; Mg-doped LATP, and zirconium -doped Li_3NbO_4);

optimize the separator coating morphology and reduce its thickness (less than 5 mm); and explore other separator coating techniques and conduct mechanical properties testing (puncture resistance, tensile strength, thermal stability, flammability, etc.). While all these sound interesting, the reviewer believed the project lacks systematic studies and a focus on fundamentals (e.g., how gradual changes in the coating chemistry and morphology affects its electrochemical properties in different electrolytes or other relevant structure-property relationships). Also, Li dendrite penetration and shortening a real cell in an EV has a very high chance to lead to a thermal runaway in the whole battery. The reviewer said that the probability of such scenarios must be reduced to the ppb level at the cell level to be commercially relevant. Increasing "cycling stability" before the dendrite shortens the cell is not sufficient to mitigate the risk of using Li-metal.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that the project addresses several points relevant to the Battery 500 goals (and more widely DOE objectives), including addressing surface reactivity of the high Ni concentration of the cathode, which will have to be addressed by a combination of cathode coating and electrolyte formulation.

Reviewer 2:

The reviewer commented that the research is closely related to DOE goals for high-energy batteries and lowering the cost. The fundamental research in this program will contribute to the accomplishment of the overall goals of Battery 500.

Reviewer 3:

The reviewer said that coatings for the cathode and separator (paid less attention before) are critical for the Battery 500 consortium team to triple the specific energy (to 500 Wh/kg) relative to today's battery technology and achieve 1,000 charge/discharge cycles.

Reviewer 4:

The reviewer found that this project, aiming at increasing cycling stability and high energy density at the cell level, supports the overall DOE objectives. The reviewer said the project has demonstrated a good balance of fundamental understanding and practical application.

Reviewer 5:

The reviewer pointed out that the projects aims to increase cell energy through exploration of new materials and processing techniques

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 PI and collaborators have fully used the resources at UW, PNNL, GM, UT-Austin, and BU.

Reviewer 2:

The reviewer found that the resources for carrying out the project appear to be sufficient.

Reviewer 3:

The reviewer said that PNNL and the Battery 500 partner institutions have sufficient resources for the proposed research.

Reviewer 4:

The reviewer noted that the Battery 500 consortium has pooled funding. The division of funds is not disclosed so no further assessment can be made.

Reviewer 5:

The reviewer said no idea, and elaborated that no information was provided for the budget of this particular project (as a part of the $10 million overall program).

Presentation Number: bat365
Presentation Title: Stabilizing Lithium-Metal Anode by Interfacial Layer
Principal Investigator: Zhenan Bao (Stanford University/SLAC)

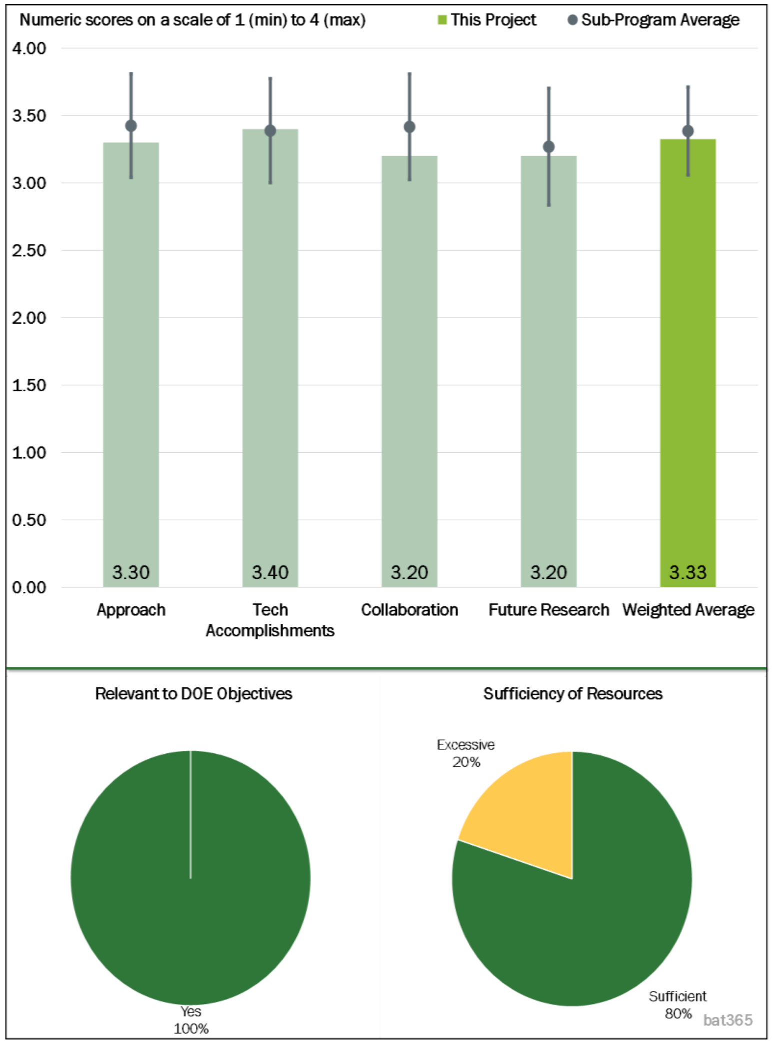

Figure 2-66 - Presentation Number: bat365 Presentation Title: Stabilizing Lithium-Metal Anode by Interfacial Layer Principal Investigator: Zhenan Bao (Stanford University/SLAC)

Presenter

Zhenan Bao, Stanford University/SLAC

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 and well-planned.

Reviewer 1:

The reviewer detailed that in this project, surface coating of the self-healing polymer has been demonstrated to be effective in improving the stability of a Li-metal anode. This project shows a good balance of fundamental understanding and practical application, via combining design/synthesis of an interfacial protecting layer with structural characterization and electrochemical testing.

Reviewer 2:

The reviewer found that the approach is rational, it addressed the technical barriers such as dendrite growth and cycle efficiency.

Reviewer 3:

The reviewer remarked that the PIs are trying to develop an interfacial layer to protect the Li-metal surface. The approach includes fundamental material investigation of the material properties, synthesis of the material, and electrochemical tests. The reviewer said that the approach aims to prevent dendrite growth and extend the cycle life of a battery with a metallic Li anode. The approach can contribute to the goals of Battery 500. The reviewer said that the PI is encouraged to engage more discussion within the Battery 500 team; e.g., polymers in aqueous environment and in Li-ion electrolyte (protic and aprotic).

Reviewer 4:

The reviewer said that this project has a multi-pronged approach at SEI layer formation and characterization. The reviewer found that the weakness is that it is too broad and viable approaches may not be able to be fully explored. The reviewer pointed out that the ability to narrowly focus on positive results will be key for this to succeed.

Reviewer 5:

The reviewer said that the project aims to produce scalable coatings on Li foils to prevent Li dendrite growth and improve CE. The reviewer was unclear though exactly how the proposed project will overcome the shortcomings of the state of the-art. The project also aims to produce "light-weight host materials with high Li affinity for the fabrication of nanoporous lithium-host composite...." The reviewer was unclear again exactly what and how the PIs aim to accomplish this and how their approach is different/superior to prior art.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer observed that significant progress has been made in surface coating with the self-healing polymer, and all the milestones were met. Improvements in the cycling stability and reduced overpotential have also been achieved through polymer coating. The reviewer said that electrochemical tests in the full cells, with general electrolyte and NMC cathodes, may be crucial for validating the proposed coating approach.

Reviewer 2:

The reviewer said that by taking advantage of extremely advanced analytical instruments, the team investigated self-healing polymers as a dynamic coating for a Li anode. The results demonstrated that the polymers can rapidly heal a pinhole, and the coating can form uniform and less-porous Li on a copper substrate. The reviewer noted that a better cycle life was demonstrated in comparison with the control anode. The reviewer encouraged the PI try to deposit thicker Li deposition on a large electrode.

Reviewer 3:

The reviewer noted that a variety of novel approaches have been developed. It looked like most of the cycle condition is mild, including the current density and the areal capacity of Li in each cycle. The reviewer recommended that the team needs to include the test with practical test conditions as well in order to further validate their approaches.

Reviewer 4:

The reviewer said that some approaches need more data to illustrate if they are possible. For example, the self-healing polymer is an interesting idea, but the permeability is not well-described. The reviewer said that more attention to the electrochemical performance including rate capability would be helpful.

Reviewer 5:

The reviewer said that the project demonstrated multiple publications in the relevant fields. The efforts have been extremely diverse and overall quite interesting, but mostly at the very early "proof-of-concept" stages. The reviewer said that it would be more beneficial for the program if the efforts were more focused/concentrated and went deeper. The reviewer said that in this case, one may expect more meaningful technology developments, including collaborations with industry/commercialization partners (even at the expense of the number of publications), or more significant breakthroughs in fundamental understanding of the relevant phenomena.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that the degree of collaboration is inherent in the Battery 500 consortium. It is a multi-pronged effort from many groups.

Reviewer 2:

The reviewer said that the PI collaborates with researchers in multiple institutions. The reviewer encouraged the PI to enhance the interactions with Battery 500 team members, especially those with electrochemistry background.

Reviewer 3:
The reviewer said that it appeared that wide collaboration within Battery 500 consortium and externally (UCLA) has been established in this project. The reviewer suggested that maybe the PI needs to state more clearly how the collaboration was carried out.

Reviewer 4:
The reviewer said that it looked as though the interaction with other teams in Battery 500 is not enough. The reviewer thought that it is necessary to make the cell with the protected Li electrode, the best positive electrode, and electrolytes from Battery 500 teams to further improve the cycle efficiency and life.

Reviewer 5:
The reviewer detailed that collaborators included Dr. Mike Toney, Prof. Jian Qin, Prof. Reinhold Dauskardt, Dr. Steven Chu, Dr. Jun Liu, and Prof. Bruce Dunn. The reviewer was unclear though what collaborator assisted in what project and how such efforts were coordinated.

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

Reviewer 1:
The reviewer said that the future work is well-stated. Electrochemical tests in coin/pouch cells under the real electrochemical conditions, as planned in this project, will be an important step to validate the polymer coating in practical use.

Reviewer 2:
The reviewer said that the PI has an adequate plan to continue her research on the polymer material for coating and Li protection. The fundamental research was also suggested to understand the interfacial phenomena on Li anode. The reviewer thought that the proposed research can contribute to reach 350 Wh/Kg goal

Reviewer 3:
The reviewer found that the proposed future work is realistic. The reviewer thought that it would be great if the team can propose more collaboration with other teams and coordinate the efforts from different aspects.

Reviewer 4:
The reviewer remarked that future goals are a little broad.

Reviewer 5:
The reviewer summarized that future research for 2018 include: elucidating the critical parameters (chemical, mechanical, etc.) for polymers; fabricating polymer coatings for coin cells testing; and fabricating new polymer membranes. Overall, the proposed studies could make sense, but the reviewer was unclear how they may provide the needed breakthroughs and how they will be different from prior art. The lack of details is not helping the reviewers.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that this project, with the goal of stabilizing the Li anode and thereby enabling high-energy density and long cycling stability of Li batteries, supports the overall DOE objectives.

Reviewer 2:
The reviewer said that the work to enhance the Li anode performance is related to the DOE goal for high-energy batteries and cost reduction. The surface coating could mitigate the dendrite growth on metallic Li anode during cycling.

Reviewer 3:
The reviewer said yes, and elaborated that Li protection is critical to achieve 500 Wh/kg and long cycle life.

Reviewer 4:
The reviewer said that the targets proposed by DOE for Li-metal anodes require novel approaches and out-of-the-box thinking to solve issues like dendrite formation.

Reviewer 5:
The reviewer said that the project aims to overcome challenges with using Li-metal anodes for fabrication of lighter and smaller 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 said that resources in this project appear to be sufficient.

Reviewer 2:
The reviewer said that the resources are sufficient considering the Battery 500 consortium already include some of the best battery researchers with broad expertise.

Reviewer 3:
The reviewer said that the combination of Stanford University and the national laboratories gives the PI more than sufficient resources to conduct her research.

Reviewer 4:
The reviewer was not clear what portion of the $10 million project went to the PI, but the reviewer assumed the resources were adequate

Reviewer 5:
The reviewer remarked that because the Battery 500 project has an overall funding, the individual project funding is not disclosed. It is difficult to assess whether individual project resources are adequate.

Presentation Number: bat366
Presentation Title: Advanced Imaging and Spectroscopic Study of Electrochemically Deposited Lithium Metal
Principal Investigator: Shirley Meng (University of California-San Diego)

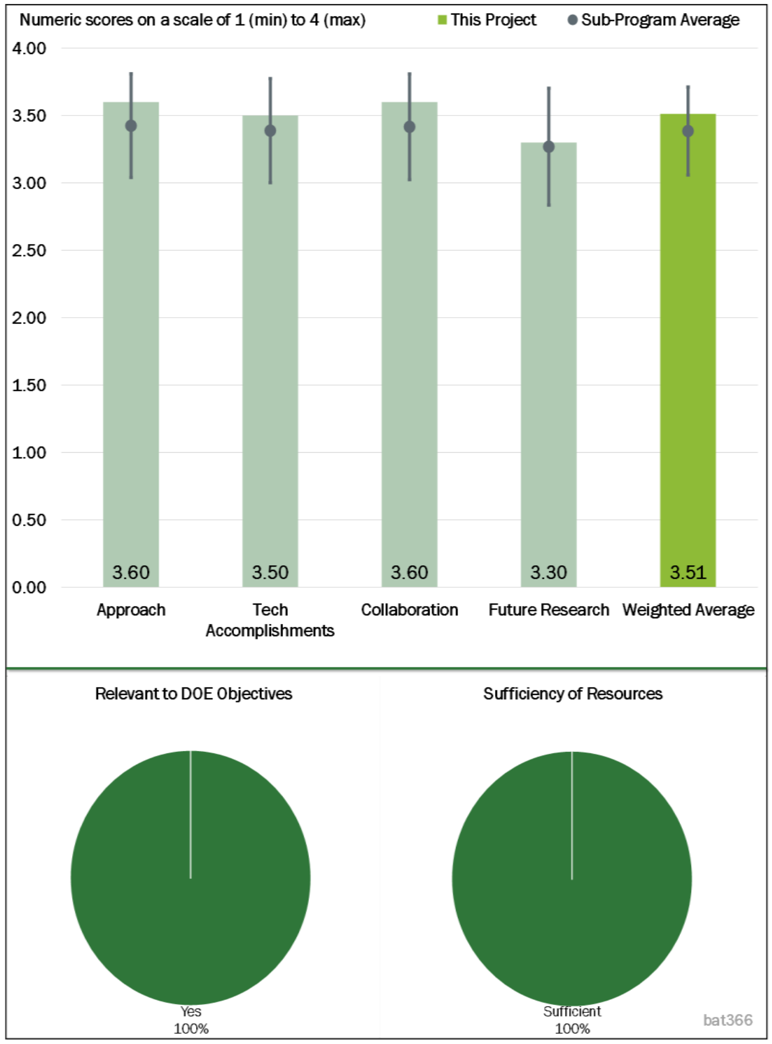

Figure 2-67 - Presentation Number: bat366 Presentation Title: Advanced Imaging and Spectroscopic Study of Electrochemically Deposited Lithium Metal Principal Investigator: Shirley Meng (University of California-San Diego)

Presenter

Shirley Meng, University of California-San Diego

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 and well-planned.

Reviewer 1:

The reviewer observed a truly outstanding approach—using cryogenic techniques clearly provides unique insights and minimal artifacts.

Reviewer 2:

The reviewer found that the approaches to the problem are laid out well. The development of cryo techniques to understand both Li-metal anodes as well as SEI layer formation will be critical going forward.

Reviewer 3:

The reviewer said that the technical barriers have been well addressed. The SEI plays a crucial role for long-term cycle stability. Understanding the nature of SEI and Li-metal would dramatically help design the system and enable low-temperature performance.

Reviewer 4:

The reviewer detailed that the project is part of the Battery 500 project, which is aiming to achieve high specific energy of 500 Wh/kg at the cell level by way of using high-capacity Ni-rich NMC oxide or sulfur cathode, combined with a Li anode. The use of a Li anode for long-life cells is quite challenging of the limited cycle life, mainly due to the Li dendrites and "dead Li." Specifically, this project focusses on utilizing the cryo-TEM to explore the nature of Li-metal and its SEI in order to improve the cycle life of Li-metal based batteries at room and low temperature. The reviewer said that to start with, electrochemically deposited lithium (EDLi) is being analyzed for its SEI in different low-temperature electrolytes. Cryo-TEM is an interesting and useful technique to examine Li and its surface conditions. The reviewer said that because of its reactivity, standard TEM cannot be used for Li. Recently, Stanford researchers reported the use of cryo-TEM commonly used for studying biological samples to examine the solid electrolyte interphase on Li and understand the interactions of Li with the interphase and captured the formation of dendrites. The reviewer thought that this technique will augment the traditional electrochemical techniques to verify the compatibility for Li-metal anode. Thus, according to the reviewer this project is well integrated with the efforts from other groups in the Battery 500 and its goals towards high specific energy of 500 Wh/kg at the cell level.

The reviewer pointed out that the dendritic behavior is exacerbated at high rates and low temperature charging. The reviewer asked if this technique is amenable to in situ studies involving low-temperature charging or rapid rate. For the ex situ studies to understand the SEI, it is not certain if the electrodes need to be washed or not.

Reviewer 5:

The reviewer observed that the approach using cryogenic electron microscope as a diagnostic tool is new in the investigation of Li anode surface and the SEI layer. The PI definitely developed a new technique to study metallic Li surface and overcome the drawback of traditional electron microscopes. The reviewer said that with the Cryo-TEM, not only the surface morphology, but also the dead Li can be investigated. The reviewer found that the approach could answer some very critical questions for the anode. The reviewer recommended that the PI should elaborate the impact of temperature change to the morphology of SEI layers.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that the project team has demonstrated the effectiveness of the technique. The PI not only successfully applied the method to investigate the metallic Li anode, but also revealed the crystal structure and morphology at of SEI layer and Li formed under different conditions. The technique is proven as a new and efficient means to investigate the mechanism and understand the electrochemical phenomena on the Li anode surface.

Reviewer 2:

The reviewer commented that the accomplishments to date are impressive for this project. The particular focus relating CE to cycle life is the basic understanding which leads to project solutions. The milestones are on schedule.

Reviewer 3:

The reviewer pointed out that the promises of the proposed approach were experimentally demonstrated. The project team confirmed that room-temperature FIB introduces additional porosity, while cryo FIB/cryo TEM shows very clean images of Li-metal and its surface. Clear differences in the deposited Li and its SEI were observed when electrolyte additives were used or when the current density changed. The reviewer cited as a quite interesting example higher current density lead to the deposition of crystalline Li, while low current density lead to the deposition of amorphous Li. The reviewer cited as another very interesting observation the correlation between the CE and porosity of the deposited Li. It would be interesting to look into the fraction of the pores occupied by the SEI and if the Li losses per unit SEI volume are affected by the electrolyte composition or deposition conditions (temperature, current, etc.). The reviewer noted that a very novel liquefied gas electrolyte at ultra-low temperature showed very high CE (99.5 stabilizing efficiency and 92% first cycle efficiency) and also dense structure of the deposited.

Reviewer 4:

The reviewer noted that good progress has been accomplished in establishing the cryo-TEM technique at UCSD. Most of the data shown here are from the reported reports of Wang, et al on the capabilities of this technique in understanding the microstructure of Li, nanostructure of EDLi and identification of the SEI, and effect of current density and electrolyte additives on the crystallinity of Li and the SEI properties. The reviewer remarked that the studies performed in this project relate to the demonstration of good cycle life in electrolytes (from ARL) with high CE forming dense Li films. The reviewer found that overall, the progress is good based on difficulties associated with these fundamental studies, utilizing this new technique, and is consistent with goals of the Battery 500 project.

The reviewer pointed out that as with other diagnostic techniques, these studies, with this interesting technique, will be more useful if it can provide any insight in the designing of new stable electrolytes for a Li anode. Also, the reviewer asked what are the stable electrolytes developed for room and low temperature use (milestone 1). The reviewer asked if these are the fluoro-methane based liquefied gases, and do they have the stability compared to organic solvents.

Reviewer 5:

The reviewer said that TEM would give only localized information. Quite often, the information is not representative. The reviewer suggested that the team might need complimentary approaches to fully understand the structure and composition of SEI.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found that collaboration is excellent, involving the key players in this field.

Reviewer 2:

The reviewer noted excellent collaborations between partners: Electrolyte studies conducted in collaboration with Dr. Jason Zhang, Dr. Wu Xu, Dr. Jie Xiao, and Dr. Jun Lu (PNNL); Dr. Kang Xu and Dr. Marshall Schroder (ARL); Dr. Boryann Liaw (INL); cryo TEM studies conducted in collaboration with Dr. Elizabeth Villa (UCSD/Biological Sciences) and Dr. Xiaoing Pan (University of California-Irvine); and the work with the liquefied gas electrolyte was conducted in collaboration with Dr. Cyrus Rustmoji (South 8 Technology)

Reviewer 3:

The reviewer said that the degree of collaboration is inherent in the Battery 500 consortium, and said that it is a multi-pronged effort from many groups

Reviewer 4:

The reviewer said that there are good collaborations with the other PIs in the Battery 500 and with Dr. Xu's group (ARL).

Reviewer 5:

The reviewer said that the PI collaborates with the Battery 500 team members and researchers of other institutions.

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

Reviewer 1:

The reviewer remarked that the future research is well-laid out and specific enough for action.

Reviewer 2:

The reviewer said that there are a few outstanding technical barriers to correlate the nanostructure of EDLi and the CE, quantify the dead (passivated) Li, and to observe the plating and stripping process of Li-metal by in situ cryo-TEM and identify electrolytes that will provide stable interface and, finally demonstrate long cycle life with Li anode in test cells. The reviewer pointed out that there are several variables that control the propensity of dendrites including the nature of electrolyte (salt, co-solvent and especially additives), current density, temperature etc., all of which need to be adequately investigated. The reviewer concluded that these studies are logical, well-planned, and consistent with the goals of Battery 500 project.

Reviewer 3:

The reviewer said that the PI proposed to further optimize the cryo-TEM technique and study metallic Li, e.g., design of new holder. By means of the diagnostic tool, the PI also proposed to investigate the SEI layer formed under various conditions, the EDLi from different conditions, etc. The reviewer found that such fundamental research can contribute in significant ways to develop high-energy Li batteries proposed by Battery 500. The reviewer wondered that without knowing the cryo-TEM in details, if a “semi in situ” technique could be developed.

Reviewer 4:

The reviewer found that the proposed research sounds very reasonable. The reviewer expressed interest in seeing the detailed studies of the SEI composition; the portion of the pores filled by the SEI; the morphology and structure of the Li and SEI after more extensive cycling in different electrolytes (regular, hydrogen-free, fluorinated, ethers versus carbonates versus others, etc.); and the effect of the electrolyte (and SEI) composition and cycling conditions on the volumetric capacity of the SEI, etc.

Reviewer 5:

The reviewer recommended that the PI needs to correlate the cycle efficiency with dead Li, and design the ideal SEI accordingly.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer detailed that for a widespread use of EVs, the batteries need to be lightweight, compact, safe, and of low-cost. The state-of-the-art Li-ion batteries are inadequate to fulfil these needs. Higher energy density and lower-cost Li-ion cells are being developed under the Battery 500 project, specifically high-capacity cathodes, either Ni-rich NMC cathodes or sulfur cathodes which need to be integrated with stable Li anodes for achieving a cell level specific energy of 500 WH/kg. The reviewer said that to achieve long-cycle life without the risk of Li dendrites requires a fundamental understanding of the SEI on Li, which this project addresses, utilizing the newly-reported cryo-TEM. The reviewer found that thus, this project quite relevant to the overall Battery 500 project and its goals.

Reviewer 2:

The reviewer found that the project is highly relevant because it looks at the side reactions, which are present within batteries containing Li-metal anodes.

Reviewer 3:

The reviewer said that all the work is in-line with DOE’s need on the developing high-energy batteries and lowering the cost. The fundamental research in this program will be better understand the mechanism of, e.g., SEI formation under different additives, dead Li, etc., which will guide the development of an effective Li anode.

Reviewer 4:

The reviewer said yes, and elaborated that SEI is an enabler for the cyclability of a Li-metal electrode.

Reviewer 5:

The reviewer commented that the project addresses very important fundamental questions related to the morphology and composition of the deposited Li and SEI using cryogenic techniques.

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 the PI has adequate resources.

Reviewer 2:
The reviewer said that the resources are adequate for the scope of the project, though the reviewer was unclear what the specific budget is for UCSD (and individual organizations in the Battery 500 project).

Reviewer 3:
The reviewer noted that the team and collaborators have strong capabilities and expertise to make the project successful.

Reviewer 4:
The reviewer was unclear what portion of the $10 million went to the PI and collaborators. The reviewer is sure it is adequate, but does not have any detailed information to judge.

Reviewer 5:
The reviewer said that since the Battery 500 project has an overall funding and the individual project funding is not disclosed, it is difficult to assess whether individual project resources are adequate.

Presentation Number: bat367
Presentation Title: Integrated Characterization Studies of Battery 500 Consortium
Principal Investigator: Xiao-Qing Yang (Brookhaven National Laboratory)

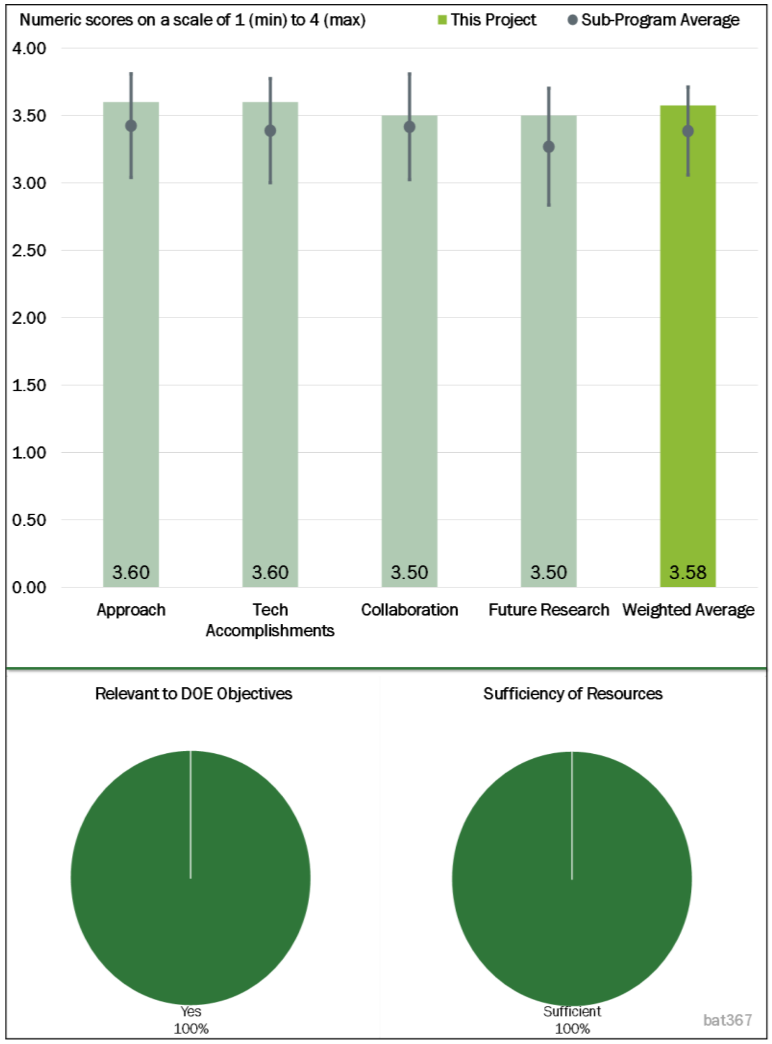

Figure 2-68 - Presentation Number: bat367 Presentation Title: Integrated Characterization Studies of Battery 500 Consortium Principal Investigator: Xiao-Qing Yang (Brookhaven National Laboratory)

Presenter

Xiao-Qing Yang, Brookhaven 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 and well-planned.

Reviewer 1:

The reviewer detailed that this project is part of the Battery 500 project being led by PNNL aiming to develop a high-capacity Ni-rich NMC cathode with higher loading and S cathodes, as well as a stable Li-metal anode to get to a cell level specific energy of 500 Wh/kg. The reviewer described that this project is dedicated entirely to performing detailed characterization studies on the Ni-rich NMC cathodes to understand the structural and compositional changes during high rate charge-discharge cycles in thick cathodes; understand the rate-limiting processes and to design new cathodes with optimized composition, doping and surface coating; understand the thermal and cyclic stability of these cathodes and to improve the energy density and rate capability of cathode materials for Li-ion batteries; and examine the SEI properties on Li-metal anodes in conjunction with different electrolytes. The project is using various advanced characterization techniques: depth-profile XRD; STEM and electron energy loss spectroscopy (EELS) to study the structural changes of Ni-rich NMC; nano-probe beamline for micro-cracks formation and propagation; HRTEM and TXM for mapping high-Ni content cycling; and synchrotron-based, soft XAS (s-XAS) and scanning transmission X-ray microscopy for characterizing the SEI. This project complements and supports the material development efforts in Battery 500 projects and is a valuable component of the overall Battery 500. The reviewer found that this project is well-designed and planned and the techniques adopted here address the key technical barriers.

The reviewer commented that undoubtedly detailed and useful characterization studies are being done here on the Ni-rich cathode. However, these (dense) electrodes designs are far from being optimized, especially for high-rate discharges causing SOC gradient across the electrode. The reviewer believed most of these techniques are in situ, otherwise there is a dilemma on whether the electrodes need to be washed or not and its impact on the SEI characterization.

Reviewer 2:

The reviewer said that the development of new ways to look at old problems is critical to move forward. The connection between the structural anomalies and the electrochemical performance needs to be more fully elucidated.

Reviewer 3:

The reviewer said that the project involved using multiple unique capabilities, including TXM (to do 3-D reconstruction for the whole particle); and s-XAS, TEM, STEM, synchrotron XRD, XPS, modeling, nano-probe X-ray microscope at hard X-ray nano-probe beamline, etc. (to explore the fundamentals of NCM failures).

Reviewer 4:

The reviewer said that the PI's approach is to use the advanced analytical techniques, e.g., micro-focused beamline, STEM, EELS, nano-probe, X-ray neutron, TXM, etc., to study the crystal structure, oxidation state, and physical structure, e.g., porosity changes of an NMC cathode material (622 and 811) during the electrochemical charge and discharge. The reviewer said that the approach is synergistically related to the research and development tasks among the Battery 500 team, because the fundamental understanding through the diagnostic analysis can guide not only the material synthesis but also the electrode developments

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer pointed out that this is the middle of second year for Battery 500 program. The PIs have made significant accomplishments. The reviewer cited as examples the inhomogeneity of SOC, oxidation of Ni, etc. of a thick NMC cathode were quantified; and the pore distribution was also identified. The reviewer said that the conclusions can not only contribute to the fundamental understanding of the NMC cathode, but also be used to guide the development of the thick electrodes, which need to be adopted for high energy density.

Reviewer 2:

The reviewer commented that the technical accomplishments are impressive, particularly all the set-ups have been installed, which would provide a tremendous capability to understand the materials.

Reviewer 3:

The reviewer detailed that the team conducted in situ depth profiling studies using synchrotron based XRD to probe the inhomogeneity of thick NMC cathodes during cycling (which was interesting and informative) and mapped (SOC distribution. By using synchrotron based nano-probe TXM imaging studies, the team observed that Ni valence state exhibits a gradient from the surface to the bulk (more Ni^2+ on the surfaces and more Ni^4+ in the bulk, which is also interesting). The reviewer cited the also-observed cation inter-mixing at charged state and proposed that it may be correlated to the reduction of Ni^4+ resulting from oxygen loss. The team also detected micro-cracks formation in bulk (as was also observed by others) and found nano-sized pores formed in the center of the particles. Finally, the results of in situ synchrotron-based XRD studies on a Li-metal anode provided information about the amount of Li consumed and dead Li formed during cycling. Overall, the reviewer found most of the findings to be very interesting and the applications of advanced techniques quite admirable.

Reviewer 4:

The reviewer said that the technical milestones are on schedule. The ability to relate current technical accomplishments to battery performance is critical for project success.

Reviewer 5:

The reviewer said that good progress has been made in characterizing the structural, phase, and compositional changes in the bulk as well as at the surface of Ni-rich cathode. As may be expected, thick electrodes exhibit inhomogeneity in composition and SOC, especially at depths greater than 75 microns, even at moderate rates of C/3. Also, as with the previous NMC cathodes, the NMC811 exhibits a gradient in Ni valence state with the surface enriched in Ni^{2+}, while the bilk consists of Ni^{4+}. The reviewer further explained that nanopores and micro-cracks seem to be developed at the center of these cathodes during cycling, and finally spinel structures appear at high charge voltages. The reviewer found that overall, the technical data gathered here over the last year and half is quite good, and the progress made is consistent with the objectives of the Battery 500 project and goals of DoE.

While the reviewer acknowledged that these studies are no doubt impressive, the reviewer speculated that these observations are the same as with NMC32 and 611, or would they be notably different for the Ni-rich materials. The reviewer asked if it would be possible to quantify the degree of these changes, to compare and contrast the NMC cathodes with different Ni content.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the degree of collaboration is inherent in the Battery 500 consortium. It is a multi-pronged effort from many groups.

Reviewer 2:

The reviewer said that there are several useful and productive collaborations ongoing with several researchers within BNL and with the Battery 500 core team, especially with PNNL, UT-Austin, BU, BNL, INL, Stanford University/SLAC, UCSD, University of Washington, and also researchers from other DOE national laboratories (ANL), the ARL, and other universities.

Reviewer 3:

The reviewer said that the PIs collaborate with almost every member in the Battery 500 teams. In addition, the project team also works with other research institutions and industry.

Reviewer 4:

The reviewer said that it shows the excellent teamwork.

Reviewer 5:

The reviewer said that the authors collaborated with all institution members of the Battery 500 consortium and with Johnson Control Inc. The reviewer suggested that it would be informative to learn more about each specific collaboration, what it involved and how it was beneficial. Additional collaboration with automotive companies (at least receiving their feedback) would also be beneficial in the future.

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

Reviewer 1:

The reviewer said that the team proposed to complete the XAS studies of the high-Ni NMC cathode; complete the TXM studies of high-Ni NMC cathode multi-cycled at high voltage charge limit to understand the effects of high voltage cycling on the performance fading; develop neutron pair distribution function (n-PDF) to study the Li-anode and electrolyte interactions; and develop and apply synchrotron X-ray based in situ XRD to study the Li stripping and deposition. Overall, the reviewer found the plans to be excellent and the reviewer is looking forward to learning about the team’s findings.

Reviewer 2:

The reviewer said that the future research, which revolves around the XAS and TXM of high-Ni cathodes with respect to high voltage cycling, should be a key piece of information to move forward with DOE objectives.

Reviewer 3:

The reviewer described that the challenges ahead for this project include developing in situ and ex situ characterization tools, e.g., synchrotron X-ray, neutron, and electron-based scattering, spectroscopic, and imaging tools to understand metal Li anode, i.e., monitor the SEI formation; the Li deposition process; the effectiveness of new additives, salts, solvents, as well as new electrolyte systems in suppressing the dendritic Li formation. The reviewer said that the proposed studies include completing the characterization of high-Ni NMC cathode multi-cycled at a high-voltage charge limit to understand the structural stability at high voltage charge and to develop nPDF to study the Li-anode and electrolyte interactions and synchrotron X-ray based in situ XRD to study the Li stripping and deposition process with different electrolytes and electrolyte additives. The reviewer said that these studies are relevant to the objectives and goals of Battery 500, are logical, and will address the key technical barriers associated with high-energy cells with Li-metal anode.

Reviewer 4:

The reviewer said that in the future, the PIs proposed to leverage the success in the investigation of the cathode and extend the techniques to metallic Li anode. The project team proposed to apply n-PDF to study the Li-anode and electrolyte interactions; develop and apply synchrotron X-ray based in situ XRD to study the Li stripping and deposition process under the conditions of various electrolyte additives; and Li/dead Li quantification. The reviewer said that the proposed work tackles the real challenges of a metallic Li anode, which is the central piece of the Battery 500 objectives.

Reviewer 5:

The reviewer pointed out that the team has proposed different approaches. For the future work, the coordination among those characterization techniques need to be further emphasized to gain a deeper understanding of the degradation mechanism, and most importantly to come up different solutions to solve the problems.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that the proposed research on the fundamental investigation of NMC cathode, Li anode, and electrode engineering, e.g., thick cathode, is critical to the development of high-energy, low-cost Li-ion batteries, which is directly related to DOE goals.

Reviewer 2:

The reviewer detailed that for widespread use of EVs and PHEVs, batteries with higher energy and lower cost than the current Li-ion batteries are needed, and the technologies based on a Li-anode with either high-capacity Ni-rich cathodes or S are expected to fulfil these needs with higher specific energy and proportionate cost benefits (from S or low-Co formulations). These high-capacity cathodes and the Li anodes have inherent technical challenges form the bulk and interfacial changes occurring during cycling, and new and advanced characterization techniques are needed to understand these changes. The reviewer found that this project is serving that purpose for the Battery 500 project and is consistent the objectives of Battery 500 and goals of the DOE-VTO program

Reviewer 3:

The reviewer commented that it appears that DOE objectives are leading to cathodes of higher Ni content operating at higher voltages. The basic understanding of structural and oxidation state changes will be necessary to determine feasibility.

Reviewer 4:

The reviewer said yes, a positive electrode is a critical component to achieve the energy density and cycle life of a Li rechargeable battery for Battery 500 goals.

Reviewer 5:

The reviewer said that the project aims to develop the advanced methodologies and gain deep fundamental knowledge needed in the development of 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 said that the PI has adequate resources to conduct the proposed research activities.

Reviewer 2:

The reviewer said that the resources seem to be adequate for the scope of the project. However, the funding information at various PIs under the Battery 500 project is not provided.

Reviewer 3:

The reviewer said that resources are sufficient, and that it would be great if the team can also include some modelling work at atomic scale to better understand the mechanism.

Reviewer 4:

The reviewer commented that because the Battery 500 project has an overall funding and the individual project funding is not disclosed, it is difficult to assess whether individual project resources are adequate.

Reviewer 5:

The reviewer could not determine if resources are sufficient (no data was provided on the budget given to this team out of the $10 million), but the reviewer assumed it is adequate.

Presentation Number: bat368
Presentation Title: Battery 500 Integrated Cell Diagnostics and Modeling to Identify Critical Gaps in Achieving High Cycle Life
Principal Investigator: Eric Dufek (Idaho National Laboratory)

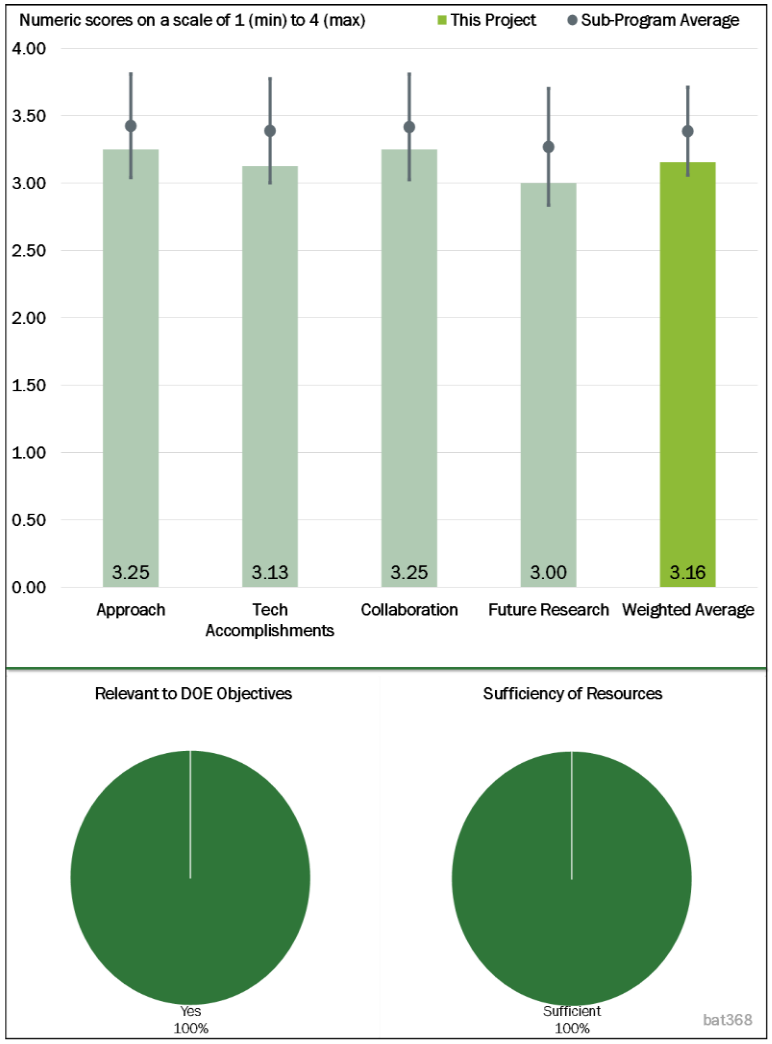

Figure 2-69 - Presentation Number: bat368 Presentation Title: Battery 500 Integrated Cell Diagnostics and Modeling to Identify Critical Gaps in Achieving High Cycle Life Principal Investigator: Eric Dufek (Idaho National Laboratory)

Presenter

Eric Dufek, Idaho 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 and well-planned.

Reviewer 1:

The reviewer said that the importance of understanding the performance space of cell designs cannot be understated. The ability to have a consistent test vehicle is important to make progress particularly in a project that includes a large number of collaborators. The reviewer noted that this eliminates the confounding nature of cell design on the measurement of electrochemical performance.

Reviewer 2:

The reviewer said that the project is part of the Battery 500 project aiming to develop a high-capacity Ni-rich NMC cathode with higher loading and S cathodes as well as a stable Li-metal anode to get to a cell-level specific energy of 500 Wh/kg. Specifically, this project is examining the cell design options, such electrode thickness and electrolyte volume to maximize the specific energy with the Ni-rich NMC cathodes. The reviewer said that both coin and pouch cell designs are being optimized to utilize the evaluation of the high-capacity materials being developed in Battery 500. The reviewer found that this project is consistent with the other Battery 500 projects and with DOE’s goals. The reviewer said that modeling would be useful in understanding the transport limitations either in thick cathodes or in cells with depleted electrolytes. However, it is not as straightforward to expect the modeling studies to provide insights into the failure modes.

Reviewer 3:

The reviewer summarized that the project involves design and modeling of cells/electrodes to guide experiment, analysis, and diagnostics; tuning the electrode microstructure, studies; and the development of the methods to quantify failure mechanism and Li transport; and finally exploring routes to improve cycle life in high-energy cells.

Reviewer 4:

The reviewer commented that theoretically, the approach was in line with the goals of Battery 500, using modeling to guide experimentation, better understanding Li anode failure mechanisms, and proposing to improve the cycle life. All of those are critical for the development of high-energy Li batteries. However, according to the reviewer the PIs really lacked a comprehensive and feasible plan, e.g., the approaches are very generic and can be applied to any Li battery projects.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that the measurement of the effect of electrode thickness and electrolyte content enables cell designs which can meet the project objectives in the Battery 500 group.

Reviewer 2:

The reviewer said that fairly good progress has been made standardizing fabrication procedures of coin cells and pouch cells, which would be helpful in evaluating the materials reliably across the different Battery 500 projects. The reviewer said that quantifying an electrolyte is crucial for Li-metal-based cells, and more so for Li/S cells to achieve adequate performance without harming the specific energy. Also, the performance of the Li/NMC (622) pouch cell, i.e., 160 cycles with the Li-metal anode, is encouraging, though the specific energy of 310 Wh/kg is not significant. The reviewer inquired if this pouch cell was fabricated at PNNL and tested here.

The reviewer posed related questions: What is consistency here, how many cells were tested, what is the spread in cycle life, and if there were there any early-stage failures common to Li cells. Further, the reviewer pointed out that adequate details are not provided in support of summary statements that analysis methods are in place to more directly correlate fade across program, and specific modeling activities were identified to focus on core areas for extending life and specific energy. Overall, the technical accomplished here over the last year and half are reasonable and the progress made is consistent with the objectives of the Battery 500 project and DOE goals.

Reviewer 3:

The reviewer pointed out that the PIs try to use Butler-Volmer equation as the core theory to model Li-ion system. Apparently, the results obtained cannot be very accurate because the model is too simplified. The reviewer could not understand the rational of the corrosion components in the model. The determinations of the sudden loss of ability for Li-ion transportation and the slow Li interfacial kinetics in a dQ/dV curves were a lack of support. The reviewer thought that the current distribution for the cathode of two different particle sizes is hard to understand. The reviewer suggested that the PIs overhaul the theoretical model; e.g., take into the consideration of ionic diffusion within the porous matrix and material with different defects or grain boundaries.

Reviewer 4:

The reviewer said that the authors observed significant cycle life reduction (by 10 times) when the team reduced the electrolyte 37 g/Ah to 6 g/Ah (not even that small as compared to commercial cells) in Li//NMC 622. The authors also introduced transport channels and reduced tortuosity. The reviewer pointed out that the authors also conducted modeling studies with dense Li-metal and porous cathodes (various particle size) and identified the need to minimize Li current density distribution to reduce Li dendrite formation. The reviewer characterized that the findings are interesting, but somewhat already known by many in the field. No major breakthroughs in technology or fundamental understanding have yet been achieved. The reviewer said that not many “out of the box” or very novel approaches have been explored.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the degree of collaboration is inherent in the Battery 500 consortium. It is a multi-pronged effort from many groups

Reviewer 2:

The reviewer said that there are good collaborations with several researchers within the Battery 500 project, especially with PNNL, and UT-Austin. Collaboration with other partners for the diagnostics may be forthcoming. The reviewer suggested collaboration with either ANL or ORNL for the pouch cell fabrication. Based on this reviewer's recollection, these two national laboratories have good experience/expertise with the pouch cell fabrication.

Reviewer 3:

The reviewer said that the PIs claim to have collaboration across the entire Battery 500 consortium. The reviewer suggested that the PIs go beyond conference calls and quarterly meetings, try to take advantage of the wide range of expertise within the consortium, so the model can be closer to reality.

Reviewer 4:

The reviewer appreciated that the team collaborated not only with multiple outside research institutions (INL, Stanford, SLAC, UT-Austin, UW, BU, UCSD, BNL) and conducted data/sample sharing, biweekly conference calls, quarterly meetings and joint publications, and also coordinated their activities with USABC, IBM, FMC, Naatbatt and Tesla. The reviewer said that it would be beneficial if the authors would clarify the contributions of each collaborator, and it would also be beneficial if the PIs would share feedback they received from industrial partners or at least specified their interactions.

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

Reviewer 1:

The reviewer said that future proposed studies to further optimize the pouch cell design for identifying Li-metal failure and understanding the impacts of non-material cell influence, perform modeling studies to accommodate new materials and cell designs, and finally to understand the failure modes for the Li/NMC and Li/S through diagnostics are relevant, logical and will address the key technical barriers associated with the high energy cells with Li-metal anode.

Reviewer 2:

The reviewer said that the proposed future work fits well with accomplishments to date. The reviewer thought that it would be helpful to produce documentation with cell design recommendations to the battery community in general to standardize both test vehicles and protocol.

Reviewer 3:

The reviewer found that the proposed future research is important to the achievement of Battery 500 overall objectives, e.g., understand the failure mechanism, better material and design for cells. However, the future research plan is too generic and lacks contents

Reviewer 4:

The team proposed to identify Li-metal failure mechanisms and the impacts of external pressure, utilize realistic cell design parameters, and further coordinate modeling efforts with the introduction of new materials and designs into coin and pouch architectures. The reviewer found that overall, such project directions make sense, but the reviewer did not see its uniqueness as many research groups around the world are exploring similar areas. The description is not very specific, making it difficult to evaluate.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:
The reviewer said that modeling the electrochemical processes in Li cells is relevant to the Battery 500 goals.

Reviewer 2:
The reviewer said that the project contributes to the development of high-energy cells.

Reviewer 3:
The reviewer detailed that for a widespread use of EVs and PHEVs, batteries with higher energy and lower cost than the current Li-ion batteries are needed, and the technologies based on Li anode with either a high-capacity Ni-rich cathode or S is expected to fulfil these needs because of the enhancements in the specific energy and expected cost benefits (from S or low-Co formulations). A robust and efficient cell design to maximize the specific energy with Li anodes and either Ni-rich NMC or S cathodes and to demonstrate high specific energy are consistent with the objectives of Battery 500 and goals of the DOE VTO program

Reviewer 4:
The reviewer said that this project is a mandatory exercise needed to guide a large consortium of scientists.

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

Reviewer 1:
The reviewer found that the resources seem to be adequate for the scope of the project. However, the funding information for various PIs under the Battery 500 project is not provided.

Reviewer 2:
The reviewer said that a national laboratory has adequate resources.

Reviewer 3:
The reviewer said that because the Battery 500 project has an overall funding and the individual project funding is not disclosed, it is difficult to assess whether individual project resources are adequate.

Reviewer 4:
The reviewer assumed resources are sufficient as no detailed budget was provided.

Presentation Number: bat369
Presentation Title: High Energy Rechargeable Lithium-Metal Cells: Fabrication and Integration
Principal Investigator: Jie Xiao (Pacific Northwest National Laboratory)

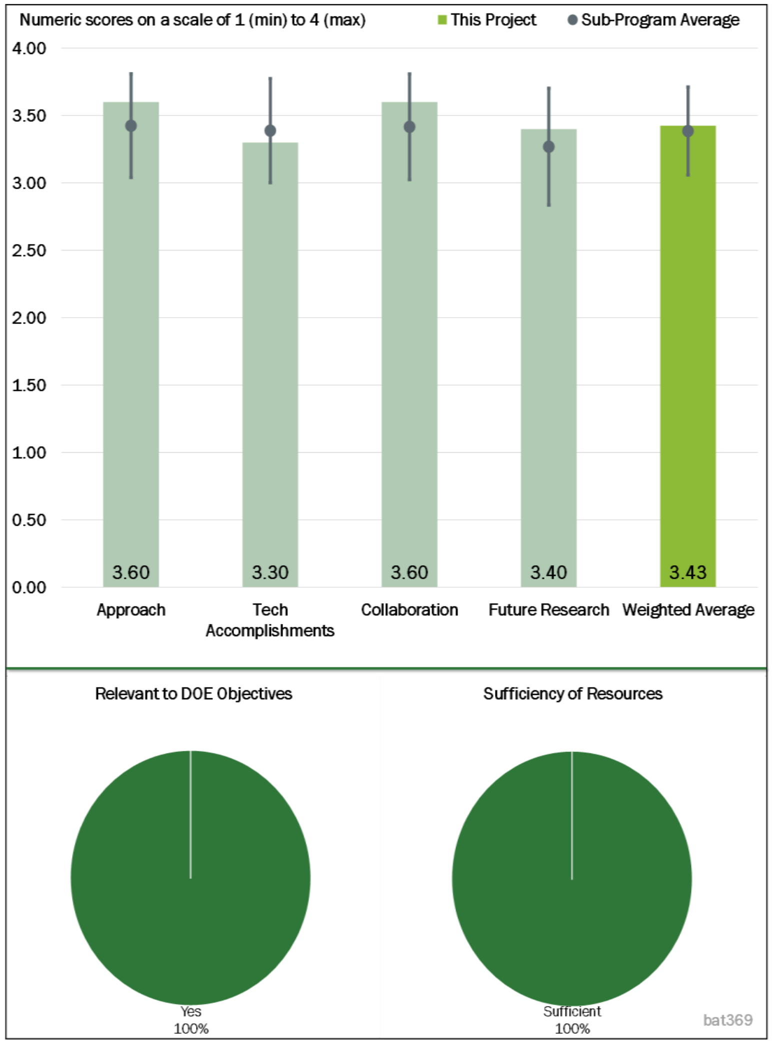

Figure 2-70 - Presentation Number: bat369 Presentation Title: High Energy Rechargeable Lithium-Metal Cells: Fabrication and Integration Principal Investigator: Jie Xiao (Pacific Northwest National Laboratory)

Presenter

Jie Xiao, Pacific Northwest 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 and well-planned.

Reviewer 1:

The reviewer said that the approaches used in this project are novel and are showing some useful results with respect to cell failure versus electrolyte amount. This complements the work by Dufek group and contributes to the chemical component of the overall cell design.

Reviewer 2:

The reviewer said that the project is well-designed by considering closing the gap between academic research and industrial application. A lot of critical factors related with battery design for achieving high-energy density have been included in the approaches. The reviewer said that quite often, those factors have not been paid enough attention in the published literature. Standardizing the testing protocol within the Battery 500 consortium is very critical to integrate the advanced technologies together to achieve the 500 wh/kg target.

Reviewer 3:

The reviewer detailed that the objective here is to address the fundamental issues in fabricating and high-energy rechargeable Li-metal cells to achieve specific energy of 500 Wh/kg. The near-term (this period) objectives are to achieve 300 Wh/kg, with Li-metal and with S or a metal oxide cathode and a cycle life of more than 50 cycles. Apart from optimizing the design and fabrication methodology for long-life Li-metal based-pouch cells, and identifying the life-limiting processes, another important task here is the development of a new electrolyte for Li anode. The reviewer said that as planned, the project is well integrated with the projects under Battery 500. The reviewer remarked that coupling with the S cathode being developed by Cui et al, or with the Ni-rich, high-capacity cathode being developed by Manthiram et al will be beneficial for the Battery 500 project. According to the reviewer, it may also be helpful to collaborate with ORNL or ANL, where there is more experience and expertise with the fabrication of pouch cells.

Reviewer 4:

The reviewer said that Battery 500 uses a unique top-down approach to revisit fundamental challenges associated with Li-metal batteries. The PI broke down all the components of a 300 Wh/kg and identified key parameters affecting the cell-level energy. The reviewer said that the areal capacity, N/P ratio, and electrolyte content are found to be drastically different with common coin cell testing and significantly affect the observed testing results. The reviewer indicated that understanding the drastic difference between coin and pouch cell structures and testing conditions will be critical to this program and discover real challenges for battery research.

Reviewer 5:

The reviewer described that the team aims to conduct analyses to understand critical issues in high-energy Li-metal cells, develop new electrolytes to extend reversible Li cycling, and understand the difference in the performance gap between coin cell and pouch cell testing. Overall, the objectives make sense, but to the reviewer it was unclear what is innovative in the approach proposed and how it is different than what is being studied in hundreds of labs around the globe.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer noted that this is the middle of the second year for this program. The reviewer acknowledged that the team has made many accomplishments. The PI successfully delivered a 300 Wh/kg Li-metal pouch cell with greater than 100 cycling (80% capacity retention). The team is also making great progress towards FY 2018 milestones, i.e., 350 Wh/kg Li-metal pouch cell with 100 stable cycling. More importantly, PNNL established standard testing protocol to close the gap between coin and pouch cell testing, which will ensure the fundamental research is conducted at relevant scale and greatly accelerate the research progress.

Reviewer 2:

The reviewer said that the progress is impressive, particularly, how to transfer the knowledge gained from coin cell to large format pouch cell. The reviewer said that this work provides the very useful guidance to academia and R&D work in industry.

Reviewer 3:

The reviewer said that fairly good progress has been made, especially in identifying the failure modes in pouch cells, standardizing the fabrication procedures for pouch cells (with limited electrolyte), and in, more importantly, developing a new electrolyte for Li anode based-cells, which shows good cycle life of ~100 cycles. The reviewer described that in most electrolytes, the SEI formed on Li anode is inadequate to protect it from further electrolyte reduction, thus resulting in a continued consumption of electrolyte and Li during cycling. Optimizing the electrolyte quantity is challenge in a Li pouch cell. The reviewer said that the new electrolyte, 1.5 M LiFSI-TEP/BTFE, seems to be more stable towards Li and is promising.

However, the reviewer asked if this electrolyte (being based on ether?) has the required oxidative stability at greater than 4V (the reviewer asked what its electrochemical window is). The reviewer also asked does the project require the development of a stable electrolyte for Li/S cells also, and is this electrolyte compatible with the S cathode and the polysulfides. The reviewer expressed surprise that the cycle life target for FY 2018 is so modest (50 cycles to 80% capacity). Overall, the technical accomplishments here over the last year and half are noteworthy and the progress made is consistent with the objectives of the Battery 500 project DOE goals.

Reviewer 4:

The reviewer found that progress towards milestones is adequate. The technical accomplishments to date have shown interesting results but need to be developed more to give a clearer picture of what Li depletion entails.

The reviewer thought that the graph showing Li depletion on Slide 10 shows an abrupt transition, which the reviewer did not expect from a chemical depletion.

Reviewer 5:

The reviewer said that the team observed dramatic expansion of Li-metal anodes after cycling and faster cell failure in pouch cells than in coin cells due to smaller electrolyte content (they all failed rapidly even at high N/P ratio of 2.6). The reviewer thought that this was an interesting observation, but many groups working with Li-metal anodes have known it for quite some time. The reviewer noted that in the course of another funded project the new electrolyte was introduced. The team used this electrolyte (1.5 M LiFSI-TEP/BTFE) and observed reduction in Li-metal swelling (compare 50 micron foils expanded to 205-320 micron after just 15 cycles in “regular” electrolyte to Li expansion from 50 micron to 150 micron in “new” electrolyte). The reviewer said that the study does not seem to be extremely systematic.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that PNNL is leading this program and has intensive interactions with all the team partners. PNNL’s leadership and coordination are the key for the program to move forward. The reviewer said that they are doing a great job.

Reviewer 2:

The reviewer said that there are good collaborations with several researchers within the Battery 500 project, specifically with the researchers from universities, other DOE national laboratories, and industry. Being a complex problem, this development will need strong collaborations in verifying the proposed cell design modifications and new electrolyte for Li pouch cells, which is being done here.

Reviewer 3:

The reviewer said that the collaboration is excellent, involving national laboratories, universities, as well as industry. The coordination across the project team and the whole teams under the Battery 500 consortium is good.

Reviewer 4:

The reviewer indicated that the degree of collaboration is inherent in the Battery 500 consortium. It is a multi-pronged effort from many groups.

Reviewer 5:

The reviewer remarked that on the positive side, the collaborative activities have been quite outstanding. In particular, the reviewer appreciated the collaboration with industry (GM) on independent testing of PNNL’s thick S electrodes and with Navitas System on a new coating method. The team also collaborated with nine universities and 3 national laboratories and clarified the nature of the collaboration very clearly.

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

Reviewer 1:

The reviewer said that future proposed studies—to further optimize the new electrolyte and separator (for Li/S) to enhance the cycling stability of Li/NMC811 and Li/S pouch cells, improve the cell design for energy density and cycle life, and finally stabilize Li anode for improved cycling—will address the key technical barriers associated with the Li anode.

Reviewer 2:

The reviewer stated that the PI has a clear plan for future research. She has a map on the pouch cell level requirements and also knows well the fundamental problems of each key component. The reviewer said that all the proposed research is directly tackling the real challenges.

Reviewer 3:

The reviewer remarked that although the proposed future work is realistic, the deliverables listed could be more aggressive based on the accomplishments achieved in last year.

Reviewer 4:

The reviewer details that the team proposes to "Demonstrate 350Wh/kg pouch cell with >50 stable cycling and <20% fading" in 2018. This may be nice, but the reviewer was unclear what exactly the team aims to focus on to overcome major barriers and how the approach is innovative and different from their peers. For 2019, the team aims to conduct optimization of the new electrolyte for Li/NMC811 and Li/S pouch cells as well as to use coated Li (e.g., produced by Hydro-Québec). The reviewer found that such description is also very general and difficult to evaluate.

Reviewer 5:

The reviewer commented that the future research for 2018 is a target but no detail is given to the approaches to that target.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The reviewer said that the project contributes to increases in stability of Li-metal cells that offer higher energy density.

Reviewer 2:

The reviewer said that all the work is directly related to DOE's need on developing high-energy batteries and lowering the cost. The fundamental research in this program will be further validated in high-energy pouch cells, which is urgently needed in battery research field.

Reviewer 3:

The reviewer described that for a widespread use of EVs and PHEVs, batteries with higher energy and lower cost than the current Li-ion batteries are needed, and the technologies based on Li anode with either a high-capacity Ni-rich cathode or S is expected to fulfil these needs because of the enhancements in the specific energy and expected cost benefits (from S or low-Co formulations). A long-life Li anode is desired to meet DOE goals, which this project has been addressing. The reviewer detailed that the project is addressing two main technical barriers for EV batteries; i.e., low specific energy with the state- of-the-art Li-ion cells partly because of the use of carbonaceous materials with low specific capacity as anode. In contrast, Li-metal anode offers many-fold improvements in specific capacity and energy, but is hampered by short cycle life of ~50 cycles due to the dendritic nature of Li deposition and passivation. The reviewer said that this project addresses these barriers by specifically addressing the challenges in fabricating suitable pouch cells to demonstrate long-life with the Li-based cells. The reviewer found that the project is well-designed and planned to develop high-energy Li cells with S or metal oxide cathodes, consistent with the goals of DOE's VTO program.

Reviewer 4:

The reviewer commented that this project along with the Dufek group is a necessary contribution to a large consortium of scientists. This sets the "chemical" design for the batteries.

Reviewer 5:

The reviewer said that the work well addressed the barrier, and proposed work is closely related with DOE targets.

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 the teams in the Battery 500 consortium are the key players in this field. Their expertise and lab capabilities are in strong position to make the project successful.

Reviewer 2:

The reviewer said that though it is not what the budget is for this particular project ($10 million for entire Battery 500), the resources seem to be adequate for the scope of the project.

Reviewer 3:

The reviewer said that national laboratories have sufficient resources.

Reviewer 4:

The reviewer said that because the Battery 500 project has an overall funding and the individual project funding is not disclosed, it is difficult to assess whether individual project resources are adequate

Reviewer 5:

The reviewer assumed resources are sufficient, although no information was provided with the budget for this particular project.

Presentation Number: bat370
Presentation Title: Advanced Diagnostics of Nickel-Rich, Layered-Oxide Secondary Particles
Principal Investigator: William C. Chueh (Stanford University/SLAC)

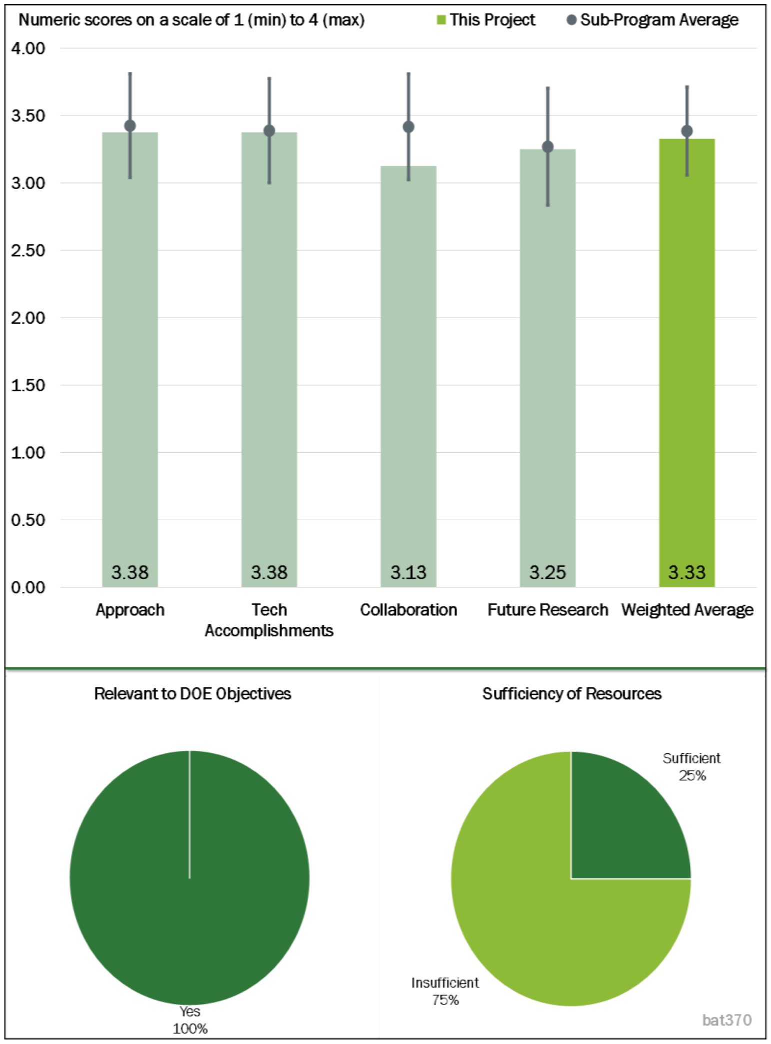

Figure 2-71 - Presentation Number: bat370 Presentation Title: Advanced Diagnostics of Nickel-Rich, Layered-Oxide Secondary Particles Principal Investigator: William C. Chueh (Stanford University/SLAC)

Presenter

William C. Chueh, Stanford University/SLAC

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 and well-planned.

Reviewer 1:

The reviewer said that the project team is developing an experimental set-up that will allow the team to measure mechanical changes to secondary particles and try to relate those data to crystallographic and electrochemical changes.

Reviewer 2:

The reviewer noted a very good and comprehensive approach to understanding fade in high-energy Li ion-cells. Excellent use of multiple diagnostics tools and good interpretation of results.

Reviewer 3:

The reviewer said that the approach taken is excellent. The PI is using a comprehensive diagnostic approach to understand the fading problems of high-Ni NMC cathodes at the atomistic through the mesoscale level. The effort is logical and appears to be well thought-out.

Reviewer 4:

The reviewer said that the project is focused on developing advanced characterization techniques to understand the chemical and microstructural changes in the electrode materials being developed in the Battery 500 project and correlate it with their cyclic stability (capacity loss), and thus guide the development of high-capacity cathodes. Specifically, the project aims to develop in situ and ex situ X-ray Spectro-microscopy technique to relate local chemistry and microstructure evolution in the cathode materials during cycling, manifesting from the electro-chemo-mechanical changes which will be probed at the relevant length-scales here. The reviewer said that these techniques are intended to correlate with other characterizations such as diffraction and electron microscopy. Thus, this project is well integrated with the efforts from other groups in the Battery 500 program.

The reviewer said that the evolution of microstructural evolution within the secondary particle due to the segmentation of the primary particles from the internal stresses due to de-lithiation would be a function of the electrolyte, which dictates the nature of SEI (or cathode electrolyte interface) on the primary particles. The reviewer thought that this study should be extended to the cathode's cycles in different electrolyte.

The reviewer pointed out that the benefit and relevance of this technique in understanding the microstructure evolution in cathodes is quite clear. The reviewer asked but how can this be extended to the imaging and diagnosis of Li-metal anode with different electrolytes and electrolytes additives, as indicated here (or it a different project in Battery 500).

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer said that this is a small project to test a new technique. The team has made quite a bit of progress with just $10,000k. The team is relying on the fact that theirs is an anisotropic change in the structure that most likely results in strain in the primary particles and between secondary particles, and their techniques can detect in terms of changes to the secondary particles.

Reviewer 2:

The reviewer said that excellent progress has been made to date. The team developed 3-D transmission X-ray microscopy to characterize the evolution of internal pore structure and cracking in Ni-rich NMC as a function of voltage and cycling. The team also developed a sectioning procedure to prepare cathode samples for analysis. The reviewer noted that surprising results have been obtained. The formation of cracks and propagation occurs on the inside. The reviewer remarked that this finding is expected to spurn additional investigations by others.

Reviewer 3:

The reviewer affirmed that good progress has been accomplished in diagnosing the Ni-rich NMC cathode and establishing through operando XRD that there is a rapid collapse of c-lattice, increasing at high charge voltages greater than ~4.2V (as known with the conventional cathodes), which is reversible but yet causes structural degradation within (secondary) particle, but no such changes on the surface. The reviewer noted the team demonstrated that the locally induced stresses and accompanying SOC heterogeneity can lead to locally overcharged domains that are detrimental the cyclic stability. The reviewer found that overall, the progress is good based on the short duration of the project and also the low level of funding for this effort.

Reviewer 4:

The reviewer noted significant amount of good results. However, the PI correlates rapid capacity fade, and it is rapid, and mechanical cracking. Typically, industry is really good at watching for this (particle cracking, electrode failure) and making sure it is not there. But the PI still has a fairly rapid fade of 811 cathodes. Cracking is certainly an issue with some NMC particles, but it is not a major issue that the PI has seen.

The reviewer saw the multi length scale chemical imaging. The reviewer said got varying SOC both from particle to particle and within a single secondary particle, which is pretty amazing. There is decent driving potential in these NMCs.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the investigator has done a good job of bringing in other institutions to get access to the equipment needed.

Reviewer 2:

The reviewer said that there appears to be good coordination between the PI, co-PIs, and collaborators for the ALS and Stanford Synchrotron Radiation Light source. It was good to see that the users' faculties were at no cost to the effort.

Reviewer 3:

The reviewer found that there are good collaborations with researchers at Stanford, but may be extended to other PIs in the Battery 500.

Reviewer 4:

The reviewer noted reasonable collaboration, and that it might be valuable for the PI to collaborate with industry a little bit.

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

Reviewer 1:

The reviewer said that this is a technique-development exploratory task. The PI is going to apply his technique to other systems to see if he can see something, like dead Li from cycling Li-metal.

Reviewer 2:

The reviewer believed that future efforts directed toward investigating cathode compositions that the Battery 500 team is pursuing is of great merit. There is no need for a thorough study of a material that will not be used. This type of support is necessary if the Battery 500 team is to meet the ultimate goals.

Reviewer 3:

The reviewer acknowledged that there are benefits in extending these studies from ex situ to in situ experiments, and to full cells to couple nanoscale electrode mapping to nanoscale crystallography in full cells. The proposed future studies will extend these studies to Ni-rich compositions investigated by Battery 500, to the cathode/electrolyte interphase chemistry, presumably as a function of electrolyte composition, using Spectro-microscopy for a quantitative understanding of the surface film and finally quantification of dead Li. These studies are logical, well-planned and consistent with the goals of Battery 500 project.

Reviewer 4:

The reviewer liked the future research, especially the quantification of the cathode/electrolyte interphase chemistry and the quantification of dead Li.

Question 5: Relevance—Does this project support the overall DOE objectives?

Reviewer 1:

The project focuses on addressing one of the major problems. The USABC and the VTO have set aggressive battery performance targets that will require higher voltage and higher energy density than present Li-ion systems. Unfortunately, one of the most promising cathode materials, high-Ni NMC, has a limited cycle life. This effort is addressing this issue.

Reviewer 2:

The reviewer noted that as we move to higher energy, everything is being pushed to its extremes. The technique will be useful in measuring changes in cells.

Reviewer 3:

The reviewer said that high-quality diagnostics are always very relevant for pointing the way forward.

Reviewer 4:

The reviewer detailed that for a widespread use of EVs, the batteries need to be lightweight, compact, safe and of low-cost. The state of art Li-ion batteries are inadequate to fulfil these needs. Higher energy density and lower-cost cathode materials are required to improve the specific energy for Li-ion cells and reduce overall cost for the battery. The reviewer affirmed that new Ni-rich cathode materials with low microstructural degradation and low performance loss during cycling are to be developed, which the present project is duly addressing.

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 resources are appropriate for the effort that is proposed.

Reviewer 2:

The reviewer guessed that the team is already spending more money than they are presently getting.

Reviewer 3:

The reviewer said that the resources seem to be inadequate for the scope of the project.

Acronyms and Abbreviations

°C	Degrees Celsius
1.5 M LiFSI-TEP/BTFE	Lithium-ion battery electrolyte
3-D	Three-dimensional
ABR	Applied Battery Research for Transportation
Ah	Ampere-hour
Al	Aluminum
ALD	Atomic-layer deposition
ALS	Advanced Light Source
AMR	Annual Merit Review
ANL	Argonne National Laboratory
ARL	Army Research Laboratory
ASIL	Automotive Safety Integrity Level
ASR	Area-specific resistance
ATR	Attenuated total reflection
BMR	Battery Materials Research
BNL	Brookhaven National Laboratory
BOL	Beginning of life
BU	Binghamton University
C	Charge rate
CAEBAT	Computer-aided engineering of batteries
CAMP	Cell Analysis, Modeling, and Prototyping Facility
CBD	Carbon-binder domain
CE	Coulombic efficiency
CEI	Cathode-electrolyte interphase
Co	Cobalt
CoEx	Co-extrusion
CT	Computerized tomography

D	Dimension
DEM	Discrete-element method
DEMS	Differential electrochemical mass spectroscopy
DFT	Density functional theory
DIC	Digital image correlation
DMC	Dimethyl carbonate
DOE	U.S. Department of Energy
DOT	U.S. Department of Transportation
E/S	Electrolyte/sulfur
EC	Ethylene carbonate
EDLi	Electrochemically deposited lithium
EDS	Electric drive system, energy-dispersive X-ray spectroscopy
EDV	Electric drive vehicle
EELS	Electron energy-loss spectroscopy
EERE	Energy-Efficiency and Renewable Energy
EES	Electrochemical energy storage
EIS	Electrochemical impedance spectroscopy
EM	Electromagnetic
EUCAR	European Council for Automotive R&D
EV	Electric vehicle
FEC	Fluoroethylene carbonate
FOM	Figure of merit
FTIR	Fourier transform infrared spectroscopy
FY	Fiscal Year
g/cc	Gram/cubic centimeter
GaN	Gallium nitride
GM	General Motors
Gr	Graphite

GWh	Gigawatt-hour
HEV	Hybrid electric vehicle
HPC	High-performance computing
HRTEM	High-resolution transmission electron microscopy
HT	Heat transfer
HV	High voltage
I_0	Exchange current
ICL	Irreversible capacity loss
INL	Idaho National Laboratory
IR	Infrared
kg	Kilogram
kW	Kilowatt
kWh	Kilowatt-hour
LATP	$Li_{1+x}Al_xTi_{2-x}(PO_4)_3$
LBNL	Lawrence Berkeley National Laboratory
LCO	Lithium cobalt oxide
LFP	Lithium-iron phosphate
LHCE	Localized high-concentration electrolyte
Li	Lithium
Li_3NbO_4	Trilithium niobate
LiEDC	Lithium ethylene dicarbonate
LiPON	Lithium phosphorous oxy-nitride
LiS	Lithium-sulfur
LLS	Layered-layered spinel
LLTO	Lithium lanthanum titanate
LLZMO	Lithium lanthanum zirconium molybdenum oxide
LLZO	Lithium lanthanum zirconate
LMO	Lithium manganese oxide

LNMO	Lithium nickel manganese oxide
LNRO	$Li_{1.2}Ni_{0.2}Ru_{0.6}O_2$
LRLO	Lithium-rich layered oxide
LTO	Lithium titanate
mAh/g	Milliampere-hour/gram
MD	Molecular dynamics
MERF	Materials Engineering Research Facility
mg/cm^2	Milligram/square centimeter
mm	Millimeter
Mn	Manganese
Mo	Molybdenum
N/P	Ratio of negative to positive electrodes
Na	Sodium
Nb	Niobium
NCA	Nickel cobalt aluminum oxide
NCM	Nickel cobalt manganese oxide
NCMA	$Li_{1.0}Ni_{0.8}[Mn, Co, Al]_{0.2}O_2$
Ni	Nickel
NMC	Nickel manganese cobalt oxide
NMP	N-methylpyrrolidone
NMR	Nuclear magnetic resonance
nPDF	Neutron pair distribution function
NREL	National Renewable Energy Laboratory
OAS	Open architecture software
OEM	Original equipment manufacturer
ORNL	Oak Ridge National Laboratory
PEO	Polyethyleneoxide
PHEV	Plug-in hybrid electric vehicle

PI	Principal Investigator
PLD	Pulsed laser deposition
PNNL	Pacific Northwest National Laboratory
PSU	Pennsylvania State University
PTFE	Poly(tetrafluroethylene)
PDVF	Polyvinylidene difluoride
R&D	Research and development
R2R	Roll-to-roll
$ROCO_2Li$	Lithium alkyl carbonate
S/cm	Siemen per centimeter
SEI	Solid electrolyte interface
SEISta	Silicon Electrolyte Interface Stabilization
SEM	Scanning electron microscope
Si	Silicon
SiC	Silicon carbide
SIMS	Secondary ion mass spectroscopy
SiO_x	Silicon oxides
SLAC	Stanford Linear Accelerator Center
SNL	Sandia National Laboratories
SOC	State of charge
SOH	State of health
SSE	Solid-state electrolyte
SSRL	Stanford Synchrotron Radiation Lightsource
SSRM	Scanning spread resistance microscopy
STEM	Scanning transmission electron spectroscopy
sXAS	Soft X-ray absorption spectroscopy
Ta	Tantalum
TEGDME	Tetraethyleneglycoldimethane

TEM	Transmission electron microscopy
TERS	Tip-enhanced Raman spectroscopy
Ti	Titanium
TiO_2-S	Titanium dioxide-sulfur
TM	Transition metal
TMPSi	Trimethoxypropylsilane
TTFP	Tris(2,2,2-trifluoroethyl) phosphite
TXM	Transmission X-ray microscope
U.S.	United States
UCLA	University of California at Los Angeles
UCSD	University of California at San Diego
USABC	U.S. Advanced Battery Consortium
UT-Austin	University of Texas at Austin
UV	Ultraviolet
V	Volt
VIBE	Virtual integrated battery environment
VTO	Vehicle Technologies Office
WBG	Wide bandgap
Wh	Watt-hour
Wh/kg	Watt-hour per kilogram
XAS	X-ray absorption spectroscopy
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction spectroscopy
Zr	Zirconium
ZrO_2	Zirconium dioxide (zirconia)