2. Batteries R&D

To strengthen national security, promote future economic growth, support American energy dominance, and increase transportation energy affordability for Americans, the Vehicle Technologies Office (VTO) funds early-stage, high-risk research. This 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 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 automated and connected 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 DOE research on the most critical research and development (R&D) barriers, and accelerate progress. The partnerships help VTO focus on research that industry 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. At the same time, VTO works with industry to ensure there are pathways for technology transfer from government to industry so that Federally-supported innovations have an opportunity to make their way into commercial application.

The Battery Technologies R&D (BAT) 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 support industry to significantly reduce the cost, weight, volume, and charge time of plug-in electric vehicle (PEV) batteries. Advanced Battery Materials Research focuses on early-stage research of new lithium-ion cathode, anode, and electrolyte materials, which currently account for 50%–70% of PEV battery cost. This work will be carried out through competitively selected, cost-shared projects, in addition to research conducted as part of the Lithium Battery Recycling Prize and National Laboratory-led Recycling Center launched in fiscal year 2019. Additionally, the subprogram will continue the Battery500 research consortium, which focuses on developing “beyond lithium-ion” technologies that have the potential to significantly reduce weight, volume, and cost by three times ($80/kWh). New research supports batteries and electrification in large trucks, which may require unique technology based on the charging patterns, daily usage, range, and overall length of vehicle life.

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 activity also supports high-fidelity battery performance, life, fast charging, and safety testing of innovative battery technologies at the National Laboratories and the lithium-ion battery recycling center.

The Behind the Meter Storage (BTMS) effort focuses on innovative solutions capable of mitigating potential grid impacts of PEV high-power charging systems, such as critical materials-free battery energy storage technologies. Solutions in the 1–10 MWh range will support optimal charging system design, eliminate potential grid impacts of high-power PEV charging systems, and lower installation costs and costs to the consumer. Efforts will include research and development of advanced power electronics and controls to assure seamless integration of energy storage, vehicle charging, and behind-the-meter power transmission.

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
bat028	Materials Benchmarking Activities for Cell Analysis, Modeling, and Prototyping (CAMP) Facility †	Wenquan Lu (ANL)	2-11	3.20	3.10	3.60	2.90	**3.16**
bat030	Cell Analysis, Modeling, and Prototyping (CAMP) Facility Research Activities †	Steve Trask (ANL)	2-16	3.70	3.50	3.70	3.40	**3.56**
bat054	First Principles Calculations of Existing and Novel Electrode Materials	Gerbrand Ceder (LBNL)	2-20	3.63	3.63	3.38	3.63	**3.59**
bat085	Interfacial Processes	Robert Kostecki (LBNL)	2-23	3.40	3.20	3.70	3.40	**3.34**
bat091	Predicting and Understanding Novel Electrode Materials from First Principles	Kristin Persson (LBNL)	2-28	3.63	3.63	3.88	3.50	**3.64**
bat164	Thick, Low-Cost, High-Power Lithium-Ion Electrodes via Aqueous Processing †	Jianlin Li (ORNL)	2-32	3.42	3.42	3.67	3.33	**3.44**
bat183	In Situ Spectroscopy of Solvothermal Synthesis of Next-Generation Cathode Materials	Feng Wang (BNL)	2-38	3.75	3.50	3.50	3.63	**3.58**
bat207	Toward Solventless Processing of Thick Electron-Beam (EB) Cured Lithium-Ion Battery Cathodes †	David Wood (ORNL)	2-41	3.30	3.00	3.30	3.40	**3.16**

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 University)	2-45	3.67	3.50	3.50	3.50	**3.54**
bat225	Model System Diagnostics for High-Energy Cathode Development	Guoying Chen (LBNL)	2-48	3.60	3.70	3.60	3.40	**3.63**
bat226	Microscopy Investigation of the Fading Mechanism of Electrode Materials	Chongmin Wang (PNNL)	2-53	3.75	3.75	3.83	3.50	**3.73**
bat230	Nanostructured Design of Sulfur Cathode for High-Energy Lithium-Sulfur Batteries	Yi Cui (Stanford University)	2-57	3.75	3.75	3.50	3.25	**3.66**
bat247	High-Energy Lithium Batteries for Electric Vehicles †	Herman Lopez (Zenlabs Energy, Inc.)	2-61	3.38	3.38	3.38	3.13	**3.34**
bat252	Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Project Completion Highlights, Part I	Jason Croy (ANL)	2-65	3.60	3.50	3.60	3.50	**3.54**
bat253	Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Project Completion Highlights, Part II	Dan Abraham (ANL)	2-69	3.50	3.50	3.60	3.75	**3.54**
bat263	PPG: Electrodeposition for Low-Cost, Water-Based Electrode Manufacturing	Stuart Hellring (PPG)	2-73	3.17	3.00	3.08	3.00	**3.05**
bat264	High-Performance Lithium-Ion Battery Anodes from Electrospun Nanoparticle/Conducting Polymer Nanofibers	Peter Pintauro (Vanderbilt University)	2-77	3.17	2.92	3.00	3.00	**3.00**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat265	Development of Ultraviolet Curable Binder Technology to Reduce Manufacturing Cost and Improve Performance of Lithium-Ion Battery Electrodes	John Arnold (Miltec)	2-81	3.50	3.33	3.08	3.00	**3.30**
bat266	Co-Extrusion (CoEx) for Cost Reduction of Advanced High-Energy-and-Power Battery Electrode Manufacturing	Ranjeet Rao (PARC)	2-85	3.08	2.83	3.42	2.70	**2.95**
bat272	Pre-Lithiation of High-Capacity Battery Electrodes	Yi Cui (SLAC)	2-89	3.17	3.25	3.25	2.92	**3.19**
bat275	Lithium Dendrite Prevention for Lithium Batteries †	Wu Xu (PNNL)	2-93	3.67	3.50	3.50	3.67	**3.56**
bat276	Mechanical Properties at the Protected Lithium Interface	Nancy Dudney (ORNL)	2-96	3.60	3.70	3.60	3.67	**3.66**
bat280	Novel Chemistry: Lithium-Selenium and Selenium-Sulfur Couple †	Khalil Amine (ANL)	2-100	3.50	3.63	3.38	3.38	**3.53**
bat282	Development of High-Energy Lithium-Sulfur Batteries †	Dongping Lu (PNNL)	2-104	3.50	3.40	3.60	3.25	**3.43**
bat286	Lithium-Air Batteries †	Khalil Amine (ANL)	2-109	3.67	4.00	3.83	3.83	**3.88**
bat293	A Closed-Loop Process for End-of-Life Electric Vehicle Lithium-Ion Batteries †	Yan Wang (WPI)	2-112	3.70	3.60	3.60	3.50	**3.61**
bat296	Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries †	Chulheung Bae (Ford)	2-116	3.50	3.38	3.38	3.25	**3.39**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat298	Efficient Simulation of Mechanical-Electrochemical-Thermal Abuse Phenomena in Lithium-Ion Batteries †	Shriram Santhanagopala (NREL)	2-120	3.50	3.38	3.50	3.25	**3.41**
bat299	Microstructure Characterization and Modeling for Improved Electrode Design †	Kandler Smith (NREL)	2-124	3.25	3.38	3.50	3.38	**3.36**
bat300	Consortium for Advanced Battery Simulation: Development of Computational Framework for Battery Analysis under Extreme Conditions †	Srikanth Allu (ORNL)	2-127	3.25	3.00	3.25	2.88	**3.08**
bat309	Electrode Materials Design and Failure Prediction	Venkat Srinivasan (ANL)	2-131	3.75	3.75	3.88	3.38	**3.72**
bat310	Advancing Solid-State Interfaces in Lithium-Ion Batteries †	Nenad Markovic (ANL)	2-134	3.10	3.30	3.30	3.40	**3.26**
bat311	Understanding and Mitigating Interfacial Reactivity Between Electrode and Electrolyte †	Dusan Strmcnik (ANL)	2-138	3.50	3.50	3.20	3.40	**3.45**
bat312	Advanced Lithium-Ion Battery Technology: High-Voltage Electrolyte	Joe Sunstrom (Daikin America)	2-143	3.10	3.00	3.00	2.90	**3.01**
bat319	Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte †	Shirley Meng (University of California at San Diego)	2-147	3.67	3.50	3.58	3.50	**3.55**
bat321	Development of Ion-Conducting Inorganic Nanofibers and Polymers †	Nianqiang Wu (West Virginia University)	2-152	3.50	3.50	3.40	3.50	**3.49**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat322	High Conductivity and Flexible Hybrid Solid-State Electrolyte	Eric Wachsman (University of Maryland)	2-156	3.70	3.60	3.30	3.10	**3.53**
bat323	Self-Forming Thin Interphases and Electrodes Enabling 3-D Structured High Energy Density Batteries †	Glenn Amatucci (Rutgers University)	2-160	3.25	3.17	2.92	2.92	**3.13**
bat326	Self-Assembling and Self-Healing Rechargeable Lithium Batteries	Yet-Ming Chiang (MIT)	2-164	3.50	3.08	3.17	3.25	**3.22**
bat327	Engineering Approaches to Dendrite-Free Lithium Anodes	Prashant Kumta (University of Pittsburgh)	2-169	2.40	2.70	2.90	2.75	**2.66**
bat328	Dendrite-Growth Morphology Modeling in Liquid and Solid Electrolytes †	Yue Qi (Michigan State University)	2-173	3.60	3.30	3.60	3.60	**3.45**
bat329	Understanding and Strategies for Controlled Interfacial Phenomena in Lithium-Ion Batteries and Beyond	Perla Balbuena (Texas A&M University)	2-178	3.13	3.13	3.25	2.83	**3.10**
bat330	Electrochemically Responsive, Self-Formed, Lithium-Ion Conductors for High-Performance Lithium-Metal Anodes	Donghai Wang (Penn State University)	2-182	3.60	3.60	3.40	3.13	**3.52**
bat332	High Electrode Loading Electric Vehicle Cell †	Mohamed Taggougui (24M Technologies)	2-186	3.00	3.13	3.25	2.88	**3.08**
bat338	Extreme Fast Charging Cell Development Overview	Venkat Srinivasan (ANL)	2-189	3.60	3.40	3.80	3.50	**3.51**
bat339	Impact of Anode Design on Fast-Charge Applications	Kandler Smith (NREL)	2-194	3.63	3.38	3.63	3.25	**3.45**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat340	Impact of Charging Protocols on Cell Degradation	Dennis Dees (ANL)	2-198	3.50	3.38	3.25	3.00	**3.34**
bat355	Development of High-Performance Lithium-Ion Cell Technology for Electric Vehicle Applications †	Keith Kepler (Farasis Energy)	2-202	3.25	3.13	3.63	3.13	**3.22**
bat356	Lithium-Ion Cell Manufacturing Using Directly Recycled Active Materials †	Mike Slater (Farasis Energy)	2-206	3.30	2.80	2.90	2.88	**2.95**
bat357	Thicker Cathode Coatings for Lithium-Ion Electric Vehicle Batteries †	Stuart Hellring (PPG)	2-211	3.13	3.25	3.50	3.00	**3.22**
bat365	Stabilizing Lithium-Metal Anode by Interfacial Layer	Zhenan Bao (Stanford University/SLAC)	2-215	3.50	3.50	3.63	3.13	**3.47**
bat370	Advanced Diagnostics of Nickel-Rich, Layered-Oxide Secondary Particles	William Chueh (Stanford University/SLAC)	2-219	3.63	3.50	3.50	3.50	**3.53**
bat371	Understanding Electrode Scale and Electrolyte Effects During Fast Charge	Andrew Jansen (ANL)	2-222	3.63	3.38	3.38	3.25	**3.42**
bat373	First-Principles Modeling and Design of Solid-State Interfaces for the Protection and Use of Lithium-Metal Anodes †	Gerbrand Ceder (University of California at Berkeley)	2-226	3.50	2-2153.25	2.75	3.33	**3.26**
bat374	Stabilizing Cathode/Electrolyte Interface by New Electrolyte Design	John Zhang (ANL)	2-231	3.30	3.30	3.40	3.20	**3.30**
bat377	Lithium-Ion Recycling Center Overview	Jeff Spangenberger (ANL)	2-235	3.80	3.50	3.80	3.50	**3.61**
bat379	Direct Cathode-to-Cathode Efforts	John Vaughey (ANL)	2-240	3.50	3.60	3.50	3.40	**3.54**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat380	Other Materials Separation	Kris Pupek (ANL)	2-244	3.38	3.38	3.38	3.50	**3.39**
bat381	Design For Recycling	Jianlin Li (ORNL)	2-248	3.33	3.17	3.50	3.33	**3.27**
bat382	Modeling and Analysis for Recycling	Qaing Dai (ANL)	2-251	3.33	3.17	3.00	3.50	**3.23**
bat383	Understanding the Impact of Local Heterogeneities During Fast Charge	Eric Dufek (INL)	2-254	3.50	3.25	3.63	3.13	**3.34**
bat386	Extreme Fast Charge Cell Evaluation of Lithium-Ion (XCEL) Batteries	Venkat Srinivasan (ANL)	2-258	3.50	3.38	3.75	3.25	**3.44**
bat387	Silicon Electrolyte Interface Stabilization Update with Question and Answer Session	Anthony Burrell (NREL)	2-262	3.50	3.38	3.63	3.13	**3.41**
bat388	Silicon Deep-Dive Update with Question and Answer Session	John Vaughey (ANL)	2-266	3.25	3.25	3.00	2.88	**3.17**
bat389	Improving the Stability of Lithium Metal Anodes and Inorganic-Organic Solid Electrolytes	Nitash Balsara (LBNL)	2-270	3.67	3.83	3.50	3.83	**3.75**
bat391	Lithiation Method for High-Energy, Long-Life Lithium-Ion Battery (L3B) †	Andrew Colclasure (NREL)	2-274	3.00	3.17	3.50	3.50	**3.21**
bat392	Enabling Rapid Charging in Lithium-Ion Batteries via Integrated Acoustofluidics †	James Friend (University of California at San Diego)	2-277	3.67	3.50	3.50	3.67	**3.56**
bat393	Development of an Extreme Fast Charging Battery †	Chao-Yang Wang (Penn State University)	2-280	3.50	3.83	3.67	3.33	**3.67**
bat394	Highly Ordered Hierarchical Anodes for Extreme Fast-Charging Batteries †	Neil Dasgupta (University of Michigan)	2-283	3.00	2.83	3.50	2.83	**2.96**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat395	Developing Safe, High-Energy, Fast-Charge Batteries for Automobiles †	Bryan Yonemoto (Microvast, Inc.)	2-286	3.38	3.38	3.63	3.38	**3.41**
bat396	Enabling Extreme Fast Charging through Anode Modification †	Esther Takeuchi (Stony Brook University)	2-289	3.10	3.20	3.40	3.00	**3.18**
bat397	Titanium Niobium Oxide-Based Lithium-Ion Batteries for Extreme Fast-Charging Applications †	Sheng Dai (University of Tennessee at Knoxville)	2-293	3.13	3.13	3.50	3.38	**3.20**
bat398	Extreme Fast-Charging Lithium-Ion Batteries †	Edward Buiel (Edward Buiel Consulting, LLC)	2-296	3.13	3.00	2.75	3.13	**3.02**
bat399	High-Quality Natural and Synthetic Graphite for Lithium-Ion Batteries †	Edward Buiel (Edward Buiel Consulting, LLC)	2-300	3.50	3.50	3.33	3.17	**3.44**
bat400	Novel Liquid/Oligomer Hybrid Electrolyte with High Lithium-Ion Transference Number (Hi-LiT) for Extreme Fast Charging †	Zhijia Du (ORNL)	2-303	3.33	3.17	2.83	3.00	**3.15**
bat401	Advanced Electrolytes for Extreme Fast Charging †	William Chueh (Stanford University)	2-307	3.38	2.88	3.25	3.38	**3.11**
bat407	Understanding and Modifying Cathode/Electrolyte Interfaces †	Jie Xiao (PNNL)	2-311	3.29	3.29	3.21	3.07	**3.25**
bat408	Interfacial Studies of Emerging Cathode Materials †	Marca Doeff (LBNL)	2-317	3.80	3.40	3.40	3.50	**3.51**
bat409	Molecular-Level Understanding of Cathode/Electrolyte Interfaces †	Mike Toney (SLAC)	2-321	3.43	3.50	3.64	3.36	**3.48**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
bat410	Developing Scanning Electrochemical Microscopy (SECM) for Cathode Interfaces †	Robert Tenent (NREL)	2-327	3.21	3.00	3.21	2.93	**3.07**
bat427	In Operando Thermal Diagnostics of Electrochemical Cells †	Ravi Prasher (LBNL)	2-333	3.30	3.30	2.90	3.20	**3.24**
bat431	Investigation on Lithium Superoxide-Based Batteries †	Khalil Amine (ANL)	2-337	3.50	3.50	3.50	3.50	**3.50**
Overall Average				**3.42**	**3.35**	**3.41**	**3.27**	**3.36**

† Denotes a poster presentation.

Presentation Number: bat028
Presentation Title: Materials Benchmarking Activities for Cell Analysis, Modeling, and Prototyping (CAMP) Facility
Principal Investigator: Wenquan Lu (Argonne National Laboratory)

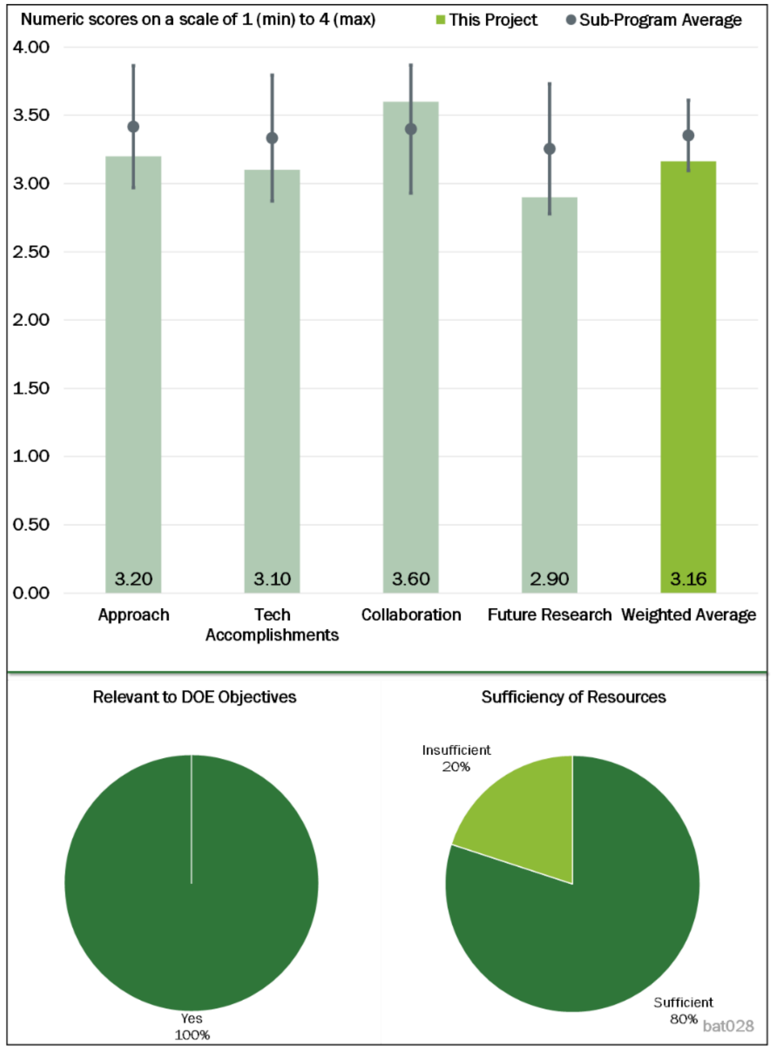

Figure 2-1 – Presentation Number: bat028 Presentation Title: Materials Benchmarking Activities for Cell Analysis, Modeling, and Prototyping (CAMP) Facility Principal Investigator: Wenquan Lu (Argonne National Laboratory)

Presenter

Wenquan Lu, 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 remarked that the project team was able to implement a rigorous approach to validation of some of the key materials such as silicon oxides (SiO_x) anodes and nickel (Ni)-rich cathodes. The reviewer said the team used sound experimental design and carefully managed testing protocols to achieve meaningful and valuable results.

Reviewer 2:

The reviewer stated that development of electric vehicle (EV) batteries that meet or exceed U.S. Department of Energy (DOE)/U.S. Advanced Battery Consortium (USABC) goals is a difficult barrier for any one project to overcome. The reviewer also stated that benchmarking is an issue that must be dealt with to facilitate the broader community to contribute to the aforementioned barrier more efficiently. The reviewer remarked the project is taking a well-designed and feasible approach to each of these issues.

Reviewer 3:

The reviewer stated that while the chemistries discussed (e.g., SiO_x, lithium nickel manganese cobalt oxide [NMC-811], lithium nickel cobalt aluminum oxide [NCA], and 90% Ni NMC) are of interest to meet the USABC goals, the testing approach was not. The reviewer noted that the electrode designs used in this presentation were low in active material content, with positive electrodes averaging 90% and negative electrodes using out-of-date polyvinylidene difluoride (PVDF) with only 92% active material. Additionally, the reviewer said the loadings are quite low such as 6.1 milligrams per square centimeter (mg/cm^2) in the NMC/NCA study. The reviewer indicated that for a facility to do valuable benchmarking work for the commercial lithium (Li)-ion industry looking to produce cells that meet the USABC goals, the electrode design needs to be one that has a chance at obtaining the goals. The reviewer suggested it would be nice to have seen the positive materials benchmarked in a greater than 95% active formulation with a loading that gives an areal capacity of more than 3 milliamp-hours per square centimeter (mAh/cm^2) and an anode with carboxymethyl cellulose (CMC) / styrene butadiene rubber (SBR) in excess of 96% active material. The reviewer suggested that for next-generation alloying materials on the negative electrode, these goals may be too aggressive, and a milder design instead could be considered should the overall electrode volumetric energy density be satisfactory to potentially meet USABC cell-level energy-density targets.

The reviewer concluded that as a benchmarking project, it is difficult to make an assessment of the studied materials, i.e., the quality of benchmarking. The reviewer asked if the selected vendors are doing something to enhance their materials, or whether this is simply a benchmark of what NCA, SiO_x, and 90% Ni are capable of relative to NMC-523/graphite. Given that some people have enabled commercial NMC-811 and some have struggled with it, the reviewer suggested it would be beneficial to understand what specifically in these materials is beneficial. The reviewer further suggested that for large-volume expansion alloys, metrics such as volume expansion could be beneficial while high-voltage or Ni-rich positive electrodes gas generation or more stability studies would be key metrics of analysis.

Reviewer 4:

The reviewer stated that pre-lithiation and high Ni cathode materials are on the right track to improve Li-ion energy density. However, the reviewer observed that there is little effort shown for cost reduction.

Reviewer 5:

The reviewer noted that the investigator demonstrated the use of best practices to benchmark screening of materials, as well as the methods being applied to enhance best practices, as is required by new and innovative materials. However, the investigator was showing a reference to USABC EV goals, which is inappropriate for the purpose of materials screening.

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 judging the research by the lofty barrier of developing EV batteries that meet or exceed DOE/USABC goals is unfair as the problem is too big for a single project. The degree of progress that has been made is excellent, though. In particular, the reviewer said, the NCA 0.9 Ni results are promising. Benchmarking accomplishments are more pronounced as the issue has been previously largely ignored. In that regard, the progress is outstanding.

Reviewer 2:

The reviewer commented that the study using Li_5FeO_4 (LFO) as an irreversible capacity loss (ICL) enrichment may be a key contribution to the battery industry. The reviewer added that it would be useful to understand the drawbacks of this approach—such as excessive gassing during formation or loss of active material content—in more detail.

The reviewer remarked that the cycle-life data are very similar to what is being shown in most other academic reports on these materials and is not novel. The reviewer further remarked that the study of the failure mechanism in the SiO_x portion is interesting but does not appear to align well with the topic of the research.

Reviewer 3:

The reviewer stated that the team was able to develop an approach to compensate for the irreversible loss of SiO_x capacity by adding cathode additives.

Reviewer 4:

The reviewer commented that because this project is now a sustaining activity, there are now more goals to implement, there is benchmarking to perform, and new methods to demonstrate results. The reviewer suggested that the project could benefit from reviewing the USABC materials targets and test methods in order to better align the materials benchmarking with the overall technology goals.

It was not yet clear to the reviewer exactly how the test results for all materials will be summarized and communicated. The reviewer encouraged the principal investigator (PI) to focus on this deliverable in the coming year.

Reviewer 5:

The reviewer stated that while there are interesting results in the report, the cell performance is behind what has been done by industry. For example, the reviewer said, industry has recognized that NMC-622/Gr or NMC-811/Gr has only 10% capacity after 500 cycles in large format full cells.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that the presentation effectively communicated how the materials benchmarking work interacts with its partners.

Reviewer 2:

The reviewer stated that the team had extensive collaboration not only within the DOE National Laboratories (i.e., Argonne National Laboratory and Oak Ridge National Laboratory), but also with large number of industrial partners.

Reviewer 3:

The reviewer found the collaboration to be excellent but added the project team should work more with industry.

Reviewer 4:

The reviewer stated it is clear that multiple National Laboratory facilities have been used in this study. The reviewer suggested that one item to improve is the test materials being sourced from foreign suppliers such as BTR, adding that there are domestic groups and suppliers of NMC, NCA, and SiO_x in the United States. Perhaps this work is on-going via the list of contributors, the reviewer wondered, but it is not ready for dissemination.

Reviewer 5:

The reviewer commented that while the project has established a wide range of collaborators, in looking through the list of industrial collaborators, there is a lack of major battery manufacturers. The reviewer said that while it may be unrealistic to expect such entities to collaborate on this project, advancing battery performance—and benchmarking even more so—would benefit greatly from their processing and materials expertise.

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 direction is adequate.

Reviewer 2:

The reviewer remarked that while future plans are generally good and well planned, some questions and observations stand out. The first question is whether SiO_x/NMC-532 cells would have a resistance to parasitic losses with additives such as fluoroethylene carbonate (FEC) or vinylene carbonate (VC). Also, the open circuit voltage (OCV) test was performed at a relativity low potential, and it would be nice to have seen a similar observation at higher energy potentials to see if the parasitic losses are exacerbated. For the second question, based on the overall capacity loss over time for a SiO_x anode in a full-cell configuration, the reviewer wanted to know whether using SiO_x as a small additive to graphite cells would address DOE lifetime requirements. Lastly, the reviewer observed that the E1 electrolyte had significantly better performance than E2 and Gen2, and it would have been nice to have seen cyclic voltammetry plots accompanied with outgas monitoring.

Reviewer 3:

Remarking that the scope of future work is ambitious for a program in year 5 of 6, the reviewer suggested that the LFO work should be the focus, specifically, understanding its drawbacks and optimizing the LFO content.

Reviewer 4:

The reviewer commented that the evaluation of high-energy cathode materials should have a specific target or purpose and added that the evaluation done in the report or proposal is a routine job for battery manufacturers.

Reviewer 5:

The reviewer referenced prior comments.

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

Reviewer 1:

The reviewer remarked that the project overall helps develop high-energy Li-ion battery technology.

Reviewer 2:

The reviewer offered that validation of battery materials is critical to achieving DOE objectives.

Reviewer 3:

The reviewer said that the project will aid in the improvement of EV performance, which is a stated DOE objective.

Reviewer 4:

Stating that there is a need for an ability to benchmark advanced materials and to generate a library of results, the reviewer encouraged continued peer review from industry partners, particularly as interesting results are uncovered, through the ongoing collaboration with advanced materials suppliers.

Reviewer 5:

The reviewer commented that benchmarking is vastly important to the development of new batteries, and that for too long, the Li-ion industry has been plagued by promises of higher energy density materials that are not true because the test was conducted incorrectly. The reviewer remarked that this project should enable better benchmarking and ensure that contributions by others to the journals is just that—contributions—and not noise that requires filtering. To that extent, the reviewer urged the project leaders to consider tightening their baselines to be aggressive and test materials in prototype cells that have meaningful parameters to achieving next-generation cell targets. The reviewer elaborated that the low loadings, high porosity, and low active-content electrodes in this presentation embody similar pitfalls that others have used that have made materials look very good but ultimately unrealistic.

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 validating materials relevant to USABC EV requirements is a fairly open-ended goal but added that funding seems sufficient to continue these activities and make an excellent contribution.

Reviewer 2:
The reviewer concluded that resources seem to be sufficient to achieve project goals.

Reviewer 3:
The reviewer commented it is sufficient.

Reviewer 4:
The reviewer did not see any evidence that resources are short and offered that the resources appear ample, but not necessarily excessive. The reviewer suggested that this project should be reviewed again in the coming year. The reviewer added that the real question will be how frequently this Cell Analysis, Modeling, and Prototyping Facility (CAMP) resource is accessed by private industry, as well as the government collaborators, and that this will help better gauge the resource need.

Reviewer 5:
The reviewer noted that the milestones listed in the presentation are not in agreement with the scope of work. The reviewer pointed out that there is no mention of work with pre-lithiated electrodes in the review but acknowledged possible limited knowledge of the full scope of this project.

Presentation Number: bat030
Presentation Title: Cell Analysis, Modeling, and Prototyping (CAMP) Facility Research Activities
Principal Investigator: Steve Trask (Argonne National Laboratory)

Presenter

Steve Trask, 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 the work has so far exhibited a great balance of best practices and adaptability to technical challenges.

Reviewer 2:

The reviewer commented that the program is very important for new materials innovation and evaluation and fills the gap between industry and academia.

Reviewer 3:

The reviewer said that the approach is effective because it enables validation of key new materials in realistic cells.

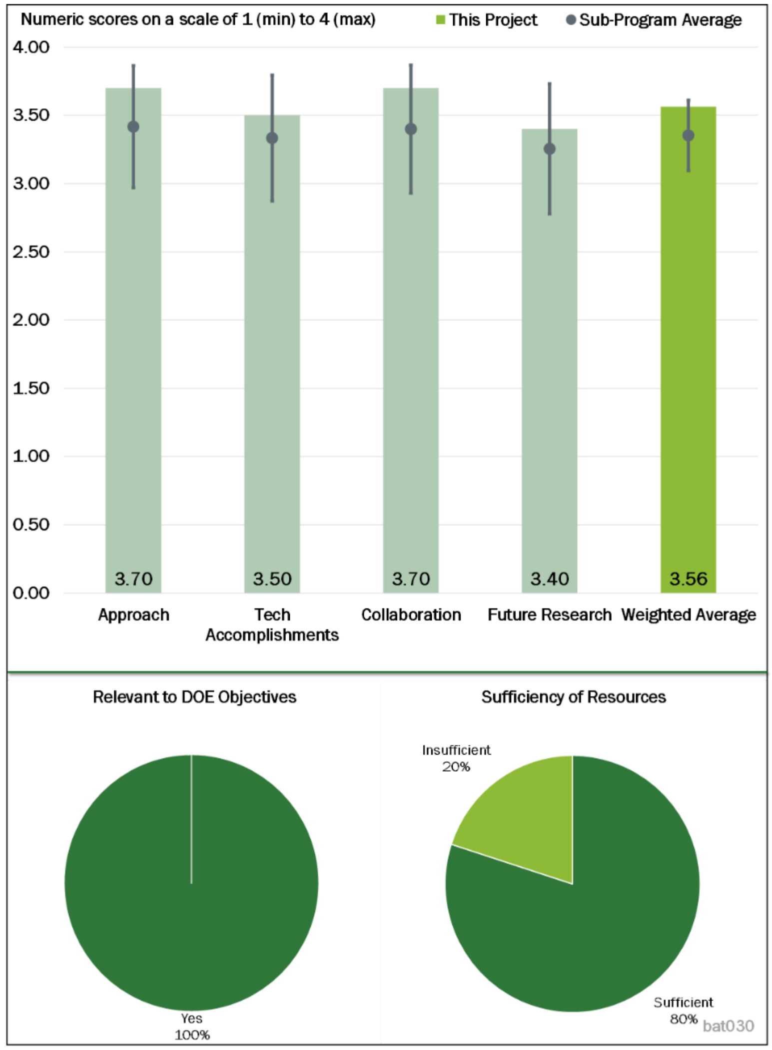

Figure 2-2 – Presentation Number: bat030 Presentation Title: Cell Analysis, Modeling, and Prototyping (CAMP) Facility Research Activities Principal Investigator: Steve Trask (Argonne National Laboratory)

Reviewer 4:

The reviewer stated that the approach is well done, adding that while the scope is broad, it is important to demonstrate the working toolbox to encourage widespread adoption of this facility and its mission. The reviewer added that one area of improvement in approach should be to ensure electrode designs are consistent with the goals outlined by the USABC. Noting that the electrode library is being developed around ~2 mAh/cm^2, the reviewer remarked that is not sufficient to achieve USABC cost or energy density targets for most near-term Li-ion chemistries. The reviewer recommended looking at expanding the library into higher areal capacity electrodes. Additionally, the reviewer observed, materials that perform well in mild electrodes may not perform well in high-energy electrodes. The reviewer concluded that providing aggressive baseline electrode designs would give a better gauge of how the material may behave in a commercial product.

Reviewer 5:

The reviewer said that Independent validation analysis of newly developed battery materials is a very important activity and one that needs to be ongoing. The reviewer remarked that technical barriers are essentially impossible to fully overcome as materials are discovered on a continuing basis, but added that nonetheless, the approach to get a grip on the issue of validation is well designed and feasible.

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 breadth and scope of the research, and in particular the ceramic coating research, are impressive.

Reviewer 2:
The reviewer said that overall the analysis technique, facility, etc., are leading-edge, adding that the topics, such as pre-lithiation, high-capacity cathode and so on, have very promising results and could impact the energy storage industry. The reviewer also said that if the analysis could be more comprehensive by working more closely with industrial companies, the results would be more valuable and practical.

Reviewer 3:
The reviewer remarked that many of the barriers involve the development and implementation of best practices but also adapting to specific innovations. The reviewer also said that progress so far appears to have been very good but that some improvements in the communication of performance indicators can be made, adding that this requires more discussion though.

Reviewer 4:
The reviewer found that good progress was made with core-shell cathode materials. The reviewer also said that while less progress has made with lithium lanthanum zirconate (LLZO) and other materials, the team has plans to accomplish those goals by year end.

Reviewer 5:
According to the reviewer, the differential scanning calorimetry (DSC) study on the core-shell materials will be an excellent study for the Li-ion industry. This highlights a key issue with these materials and how they behave in thermal abuse. It is important that this work is published as many researchers are focused on coatings for nickel-rich NMC materials and claim safety, but this study shows that surface modification via core shell only provides capacity stability and not thermal stability. The coating work is also interesting to the reviewer, but given the challenges in producing a uniform quality coating, it is too early to determine its benefits.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the team worked extensively with DOE National Laboratories and also some industrial partners.

Reviewer 2:
The reviewer found that the collaboration is well organized and that certain collaboration with industrial should be encouraged.

Reviewer 3:
Noting that it is evident that this team is utilizing multiple National Laboratories and personnel, the reviewer remarked that this sort of collaboration is key to producing quality data as it ensures key test parameters are consistent across groups and promotes standardization that this field has lacked for a significant time. The reviewer encouraged better interaction with cell manufacturers. The reviewer also remarked that while it may be challenging due to multiple non-disclosure agreements (NDAs), things that could be accomplished in a semi-blind study may provide honest feedback and potentially bring technologies to market more quickly.

Reviewer 4:

The reviewer remarked that all evidence indicates that the exact collaboration goals needed for this kind of project have been met. The reviewer added that the electrode library and how it will be used will play a useful gauge as to how well the program collaborates on the feedback side.

Reviewer 5:

The reviewer said the list of collaborators is impressive; however, the inclusion of some major battery manufacturers, if possible, 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 improving the coating method is an excellent next step. The reviewer added that given that this project is close to the end time, it is key that the project team complete the necessary work to ensure that the coatings can be well tested.

Reviewer 2:

The reviewer commented that, in general, the planned future work is excellent. Additionally, the reviewer questioned what effect, if any, the ceramic films have on the first and subsequent cycle Coulombic efficiency (CE) and whether the added thickness of a ceramic separator compared to polymer separator is worth the loss in energy density.

Reviewer 3:

The reviewer stated that there is a good plan forward for some areas, including the ability to service solid electrolyte work.

Reviewer 4:

The reviewer found that the proposed future research continues to address the barriers and moves on the track to commercialization.

Reviewer 5:

It made sense to the reviewer to focus on slurry rheological effects and roll-to-roll coating in future work.

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

Reviewer 1:

The reviewer agreed that the project contributes to the development of high-energy EV Li-ion batteries, from leading-edge materials to processing techniques, and that it well supports the DOE objectives.

Reviewer 2:

The reviewer remarked that this project is supporting all other DOE battery research projects by ensuring small-scale experiments translate into meaningful results in larger prototype cells that better reflect performance in commercial cells. The reviewer added that this is a key gap missing in many start-ups and grant-funded research projects due to the high initial equipment cost of Li-ion cell prototyping and the expertise required to be successful. This reviewer also said that this feedback will enable other DOE project teams to ensure they are producing meaningful results that can lead to commercial successes. The reviewer encouraged the PI and participants to continue to expand this effort and promote standardization in testing and providing proper test cells to smaller groups.

Reviewer 3:
The reviewer stated that cell testing and modeling are critical to achieving DOE objectives.

Reviewer 4:
The reviewer said that the research will substantially contribute to the improvement of EV batteries, a DOE objective.

Reviewer 5:
The reviewer commented that the PI needs to be cautious about the degree to which cell design optimization efforts creep into the work, because it does not appear that this should be part of the research scope.

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

Reviewer 1:
Funds appeared to the reviewer to be sufficient to continue the activity at the excellent pace to date, providing valuable validation of materials to enable the research community to more efficiently pursue DOE battery goals.

Reviewer 2:
The reviewer said that resources are sufficient.

Reviewer 3:
Resources are adequate, according to the reviewer, who stated that this is a cost-effective program because most of the expensive novel research is being streamed into this project from other programs.

Reviewer 4:
Finding that no evidence was seen that there are issues with resources, the reviewer suggested the PI consider a way to show metrics that indicate how quickly a project turn-around is done and what a reasonable turn-around time should be (based upon an assumed start of program level of complexity). The reviewer added that this may help in tracking both resources and performance.

Reviewer 5:
For such a big team, the reviewer commented, the size of funding seems insufficient to move the proposed work fast enough.

Presentation Number: bat054
Presentation Title: First Principles Calculations of Existing and Novel Electrode Materials
Principal Investigator: Gerbrand Ceder (Lawrence Berkeley National Laboratory)

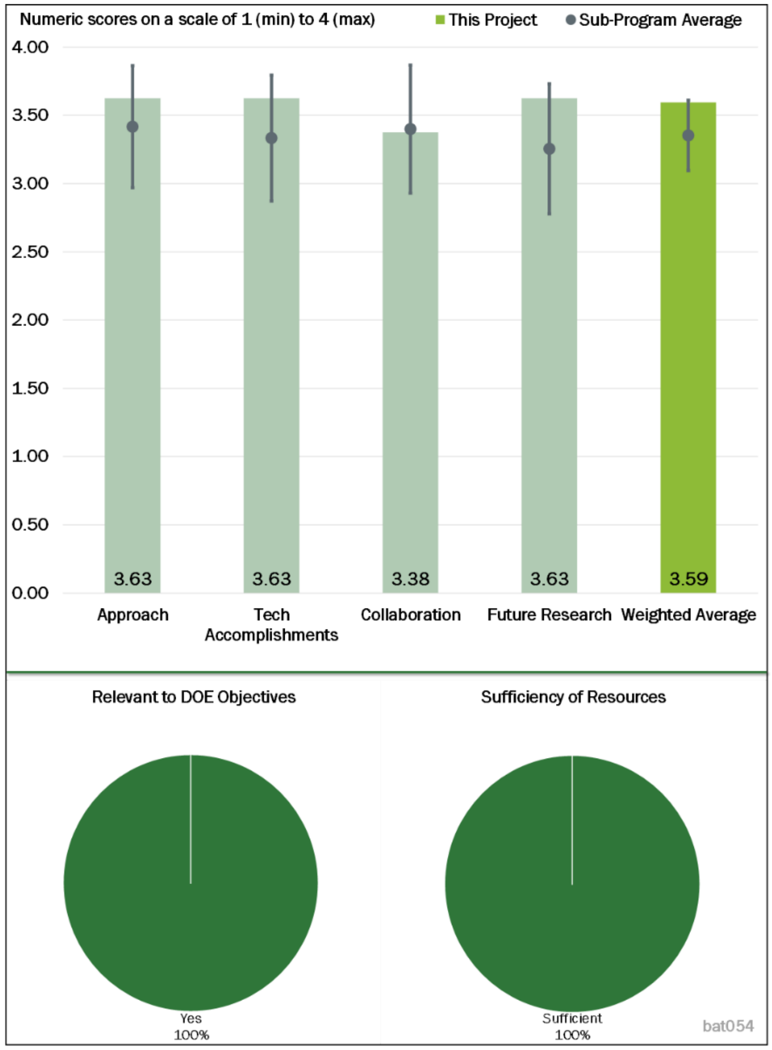

Figure 2-3 – Presentation Number: bat054 Presentation Title: First Principles Calculations of Existing and Novel Electrode Materials Principal Investigator: Gerbrand Ceder (Lawrence Berkeley National Laboratory)

Presenter

Gerbrand Ceder, 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 remarked that the approach is very strong, adding that first-principle investigations are a proven way to understand fundamental mechanisms at play in materials.

Reviewer 2:

The reviewer stated that technical barriers, such as ionic conductivity of the solid-state electrolytes as well as correlation between synthesis condition and performance of Li-thiosulfate conductors, are addressed very well, and the progress made in the project clearly demonstrates its good design and feasibility.

Reviewer 3:

The reviewer commented that the approach used is good for high throughput screening of candidate coatings for lithium phospho-sulfide (LPS) compound systems and stability of LPS phases, adding that an approach for predicting amorphous structures has been proposed. The reviewer also noted that while the interface coating approach is good, it could miss some stability problems due to the approximations used in the high throughput method.

Reviewer 4:

The reviewer stated that this program has deviated from the initial work. Initially, the disordered rock salt cathodes were a focus, but the reviewer noted that was transferred to a different program; this work instead focuses on solid-state ion conductors. Currently, the reviewer observed, work has been done to model the phase diagram for the LPS system and investigate different coatings to help with the cathode-electrolyte interface. The reviewer said the project team showed a nice graph that compares LPS reactivity and the reactivity with NMC and came out with several coatings that could help with 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 stated that excellent accomplishments are reported for all three areas of research on LPS solid conductors, i.e., bulk phases, coatings, and amorphous, adding that all the results are among properties needed for understanding and designing these solid electrolytes. The reviewer concluded that the work contributes to overcoming many barriers to use of this type of solid electrolyte.

Reviewer 2:
The reviewer said that all technical accomplishments are relevant and stay in line with scheduled milestones. The reviewer praised the results obtained for amorphous LPS using an ab-initio molecular dynamics (MD) approach as outstanding and very useful for designing novel Li-ion conductive solid-state electrolytes with targeted conductivity of about 1 milli-Siemen per centimeter (~10^{-3}S/cm). This reviewer concluded that this work is definitely addressing the key technical barriers of the Li-ion solid-state batteries.

Reviewer 3:
The reviewer found that good correlation was established between the phase diagram for and the local structure of thio-sulfate conductors and conductivity, adding that it is critical to identify good coatings as these sulfates are often not stable above 2.5 volts (V) or at Li-metal potentials.

Reviewer 4:
The reviewer said that with the limited time given for the new study, the project team has not been working on the solid-state ion conductors long, but that in that time, the project team has been able to give some important insights into the amorphous and crystalline nature of LPS. Additionally, the reviewer said, the project team has shown good work on LPS reactivity with different coatings to help with the interface with the LPS and the cathode material.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said the project team has been collaborating with Lawrence Berkeley National Laboratory (LBNL) and such a collaboration is very productive.

Reviewer 2:
The reviewer stated that the project team has worked well to accomplish the goals and objectives.

Reviewer 3:
The reviewer found good collaboration on the project team, but it would be good to have seen more interaction with experimentalists who can test the predictions of these models and test the resulting materials in full cells.

Reviewer 4:
The reviewer observed that the project team is quite small and located only at 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:
Finding the proposed future work well planned, the reviewer said the project team will focus on several key tasks such as the fundamental understanding of the mechanism of ionic conductivity in amorphous LPS and, based on that knowledge, develop a rational design strategy for significant improvement of the ionic

conductivity in this class of solid-state conductors. The reviewer also said the proposed future work seems logical and makes perfect sense.

Reviewer 2:

The reviewer said there is appropriate future research and it is very strong.

Reviewer 3:

The reviewer commented that the project team has a good proposed future research plan that is effective.

Reviewer 4:

The reviewer remarked that the plans for future work are mainly on amorphous LPS with some work planned on the evolution of conductivity of LPS at different compositions and phases. The plan to focus on understanding amorphous materials is a good one as it may have some advantages. The reviewer remarked that the planned work can help overcome some potential barriers for use of amorphous materials.

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

Reviewer 1:

The reviewer said the project is highly relevant and directly supports Vehicle Technologies Office (VTO) goals. The reviewer elaborated that the design of solid-state batteries with low price, high energy density, and excellent cyclability are the main VTO program objectives, and the present project contributes much into achieving these challenging goals.

Reviewer 2:

The reviewer stated it is extremely relevant.

Reviewer 3:

The reviewer observed that understanding how to prepare better LPS solid-ion conductors that are stable and non-reactive with the coatings for the cathode are important and added that the project team has shown relevant parameters for this.

Reviewer 4:

The reviewer commented that the project supports the overall objectives of DOE to develop electric vehicles for energy conservation, and that it fits in well with the Advanced Battery Materials Research (BMR) objectives for solid-state electrolyte (SSE) 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 found that the project team has sufficient financial, computational, and human resources to complete the project in a timely manner.

Reviewer 2:

The reviewer said resources are reasonable and are providing very good value for DOE investment. The reviewer suggested considering an increase in resources to enable more interaction with experimental groups.

Reviewer 3:

The reviewer stated that the team has shown relevant resources for the project.

Reviewer 4:

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

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

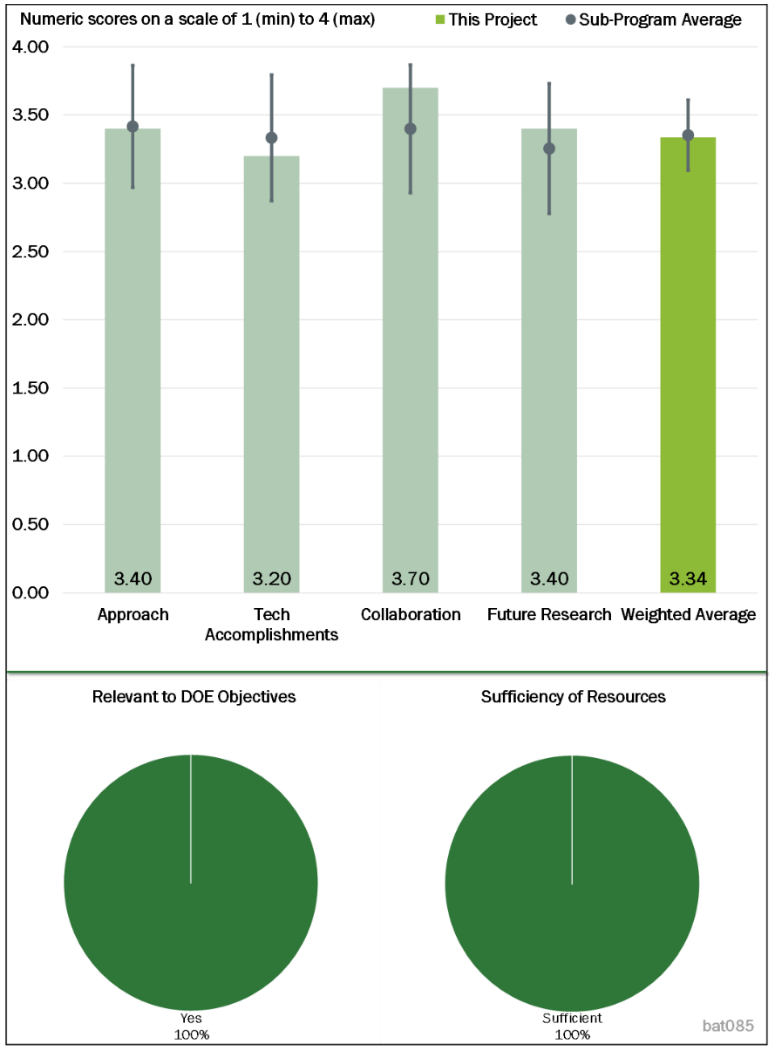

Figure 2-4 – Presentation Number: bat085 Presentation Title: Interfacial Processes Principal Investigator: Robert Kostecki (Lawrence Berkeley National Laboratory)

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 explained that the approach taken by the project team revolves around the development of advanced in situ and ex situ characterization techniques to study the electrode-electrolyte interface in Li-ion, lithium-sulfur (Li-S), and Li-metal batteries. The reviewer elaborated that the proposed in situ and ex situ characterization techniques will help to determine the interface kinetics, interphase formation, and battery degradation mechanism in real time. The reviewer concluded that the system chosen by the project team is very appropriate for the current DOE project, mainly to solve the issue of polysulfide (PS) dissolution in a sulfur-based system and solid electrolyte interphase (SEI) formation in a Li-metal battery.

Reviewer 2:

The reviewer stated that the work is mainly focused on demonstrating the use of polyethylene oxide (PEO) units in binders to suppress PS loss to the electrolyte. The reviewer added that the percentage of PEO content is carefully controlled and the experiments, from dissolution to spectroscopy and electrochemistry, are well designed.

Reviewer 3:

While praising the nice approach of applying existing, and developing novel (Kerr-gated Raman), diagnostics techniques, the reviewer was less convinced that the design of new co-block polymer binders for Li-S cells will be valuable. This chemistry is so far from commercialization that a long leash is perhaps appropriate. The reason the reviewer is skeptical is that tying up PS so that they do not poison the anode, which is being attempted here, will reduce the watt-hour per kilogram (Wh/kg) of the cell because all of the PS trapping is being done by non-active material.

Reviewer 4:
The reviewer remarked that the electrode-electrolyte interface is a tough subject to attack. Observing that most ex- situ techniques might lead to the unintentional chemical and morphological change on the interface during processing, the reviewer concluded therefore that in situ techniques are highly desired to investigate the properties of a functioning interface.

Reviewer 5:
The reviewer explained that the project is using ultraviolet (UV)- visible spectroscopy, in operando X-ray absorption spectroscopy (XAS), ex situ X-ray photoelectron spectroscopy (XPS), and Kerr-gated Raman spectroscopy to investigate the new co-block polymer binders for Li-S batteries, and that these approaches provide chemical information on electrolyte and surface-sensitive information on sulfur-composite electrodes. The reviewer would like to have seen more results on electrodes with new co-block polymer binders (PEO-PS) by using Kerr-gated Raman spectroscopy. The reviewer suggested it would be better if chemical and structure information on S cathode and Li interfaces can also be provided along with impedance measurement.

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 effect of PEO binding with PS is clearly established, elaborating that S K-edge XAS and XPS measurements are very effective in complementing electrochemical and optical data. While the Kerr-gated Raman spectroscopy is still preliminary, the reviewer added, the observations of hexafluorophosphate (PF_6) species are very interesting.

Reviewer 2:
The reviewer noted this study focuses on the application of the new spatially resolved in situ and ex situ characterization techniques to develop a detailed understanding of both structural and dynamic aspects of electrode-electrolyte interfaces in Li-S and Li-metal batteries. The reviewer also explained that sulfur K-edge XAS and XPS measurements of the electrolyte and Li-anode reveal that the presence of PEO-PS (65:35 weight percent [wt.%-) binder in the S composite cathode suppresses Li polysulfides formation and dissolution. The PIs also carried out proof-of-concept Kerr-gated Raman experiments for the first time to investigate electrolyte degradation processes in Li--metal and Li-ion batteries. Lastly, the reviewer explained that ex situ and in situ Kerr-gated Raman characterization can unravel the fundamental reaction pathways at the electrode-electrolyte interfaces of battery systems, which will definitely help in designing new materials architecture and surface stabilization efforts of existing materials.

Reviewer 3:
The reviewer pointed out that two pieces of work were presented under this project and that a detailed investigation on the impact of binder on the dissolution of Li polysulfides was conducted, adding that convincing evidence on the positive impact of PEO-based binders was clearly delivered. However, the fundamental understanding on why PEO is better than PVDF was not clear to the reviewer. At the same time, some preliminary work on Kerr-gated Raman spectroscopy to detect fluorescent species in Li and Li-ion batteries was presented. The reviewer concluded that the high sensitivity of this technique can be valuable for the community.

Reviewer 4:
The reviewer remarked that good progress has been accomplished in this project, elaborating that the new co-block polymer binders presented in this project show better CCE than PVDF and PEO-PS electrodes after 150 cycles. The reviewer also explained that this project identifies a potentially good binder: PEO-PS (65:35) to suppress Li-polysulfide formation and dissolution by using XAS and XPS analysis. The progress is good, the reviewer said, but added that the project timeline and milestone were not clearly shown.

Reviewer 5:
The reviewer stated that accomplishments to date on co-block polymer binders for Li-S have resulted in relatively minimal cycle-life improvement.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found excellent collaboration with multiple university and commercial partners and was very impressed with this fact as it helps to ensure the research is well focused and relevant to industry needs.

Reviewer 2:
The reviewer stated that the group at LBNL has an excellent collaboration in the National Laboratory network and, additionally, has interactions with United Kingdom (UK) universities and two companies.

Reviewer 3:
The reviewer commented that the PI has good collaboration with other national user facilities and universities, and that the PI also collaborates with a laser facility in the UK.

Reviewer 4:
The reviewer said that the team has broad collaboration with other teams under the Advanced BMR program, as well as university and industrial partners.

Reviewer 5:
The reviewer noted that the project has a single PI who is apparently working closely with other Advanced BMR teams.

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 research on pre-forming a Li-metal film as an artificial SEI looks extremely valuable. The reviewer was glad to see that the block-co polymer work on Li-S cells is not part of future work.

Reviewer 2:
The reviewer noted that future efforts mainly focus on development of in situ XPS and near-field infrared (IR) spectroscopy to study the Li electrode-electrolyte interface and real-time electro-kinetic measurements on gaining a deep understanding of complex electrochemical processes occurring at the electrode-electrolyte interfaces. The reviewer also indicated that future efforts to work with Advanced BMR and industry partners to establish clear connections among diagnostics, theory and modeling, materials synthesis, and cell-development efforts could lead to the development of strategies mitigating the PS dissolution and SEI formation. The reviewer concluded that these efforts will definitely result in progress in the very demanding electrode-electrolyte interface characterization field.

Reviewer 3:
The reviewer stated that the PI proposed to perform electrode surface treatment and characterization on electrolyte-electrode interfaces. Also, the reviewer explained, in situ time-resolved XPS and near-field IR spectroscopy are proposed to investigate reaction kinetics and dynamics, which are quite important for the development of Li-S batteries.

Reviewer 4:
The reviewer provided two points: First, the proposal to work on the Li interface is vague. There is no clear message on either the "preform" approach or the technique to study the interfacial phenomena. Second, there are good proposals to develop advanced diagnostic tools for battery research, noting that further development of Kerr gated Raman spectroscopy was mentioned, assuming this work will be finished in fiscal year (FY) 2019.

Reviewer 5:
The reviewer stated that this project has proposed to move to study Li-metal using techniques including in situ XPS and near-field IR spectroscopy. The reviewer noted that the PI also argued for the importance of developing non-steady techniques that can capture kinetics and dynamics. While both of these are worthy goals, the reviewer said the PI did not provide a justification for moving away from PS work, which remains very challenging and deserves continued attention, adding that the PI could also be more specific about how each technique is uniquely suited to answer what specific questions related to Li and S electrodes.

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

Reviewer 1:
The reviewer agreed that this project greatly supports DOE VTO efforts to develop high-performance and high-energy density batteries.

Reviewer 2:
The reviewer found that the project is highly relevant to overall DOE objectives, which are aimed to at developing high-energy batteries with lower cost. The reviewer added that a fundamental understanding of interfacial reaction will be necessary to determine the feasibility of the application of Li-S batteries in EVs.

Reviewer 3:
The reviewer responded that both Li-electrode chemistry and PS chemistry are highly critical for the development of Li-S batteries, which are an important technology for energy storage that has the potential for low cost, high energy density, and no need for critical materials.

Reviewer 4:
The reviewer stated the project is highly relevant because nearly all critical performance issues in Li-ion and Li-battery systems arise at the interface. The reviewer added that expanding our tool set and our analyses for interfaces is critical for enabling next-generation energy storage. Also, the reviewer said, Li-S cells are one of the few chemistries that will give us the energy density and material supply that is needed for full EV adoption.

Reviewer 5:
The reviewer explained that the research project outcomes will lead to increasing the fundamental knowledge of SEI chemistry of Li-metal battery systems and will increase the ability to design advanced materials for long cycle life and to achieve the DOE-targeted energy density without performance degradation.

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 very good value for the research and development (R&D) funding investment.

Reviewer 2:
The reviewer said the resources are adequate for the scope of the project.

Reviewer 3:
The reviewer agreed that the PI has adequate resources to conduct the proposed research.

Reviewer 4:

The reviewer stated the support level is adequate for a project that deals with method development and application to specific examples, adding that collaboration with other teams can maximize the impact of the work.

Reviewer 5:

Commenting that the milestones were not presented, the reviewer assumed that resources are sufficient for the work.

Presentation Number: bat091
Presentation Title: Predicting and Understanding Novel Electrode Materials from First Principles
Principal Investigator: Kristin Persson (Lawrence Berkeley National Laboratory)

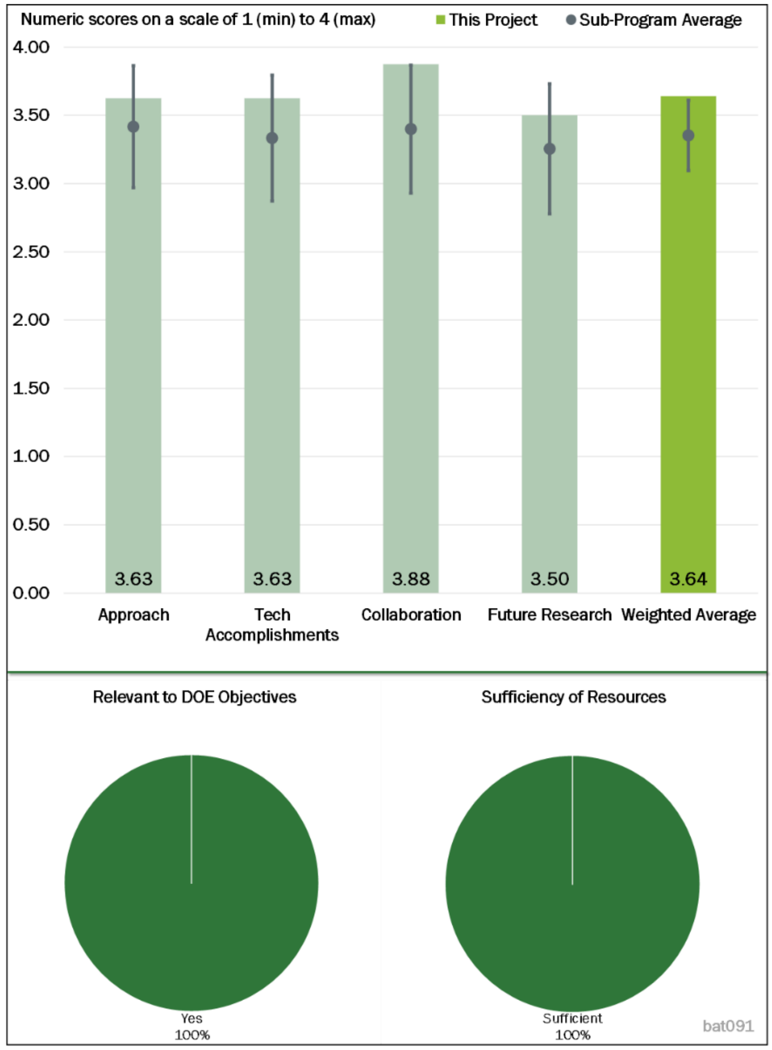

Figure 2-5 – Presentation Number: bat091 Presentation Title: Predicting and Understanding Novel Electrode Materials from First Principles Principal Investigator: Kristin Persson (Lawrence Berkeley National Laboratory)

Presenter

Kristin Persson, 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 said technical barriers, such as Li-ionic conductivity in non-aqueous, super-concentrated electrolytes as well as Li-ion conduction in silicon (Si) alloy anodes are well addressed, and the progress made in the project clearly demonstrates its good design and feasibility.

Reviewer 2:

The reviewer found that various approaches used in this project are very good, including classical molecular dynamics and density functional methods, adding that these are applied to various sized systems, as needed, in different projects. The reviewer said that potentials used for the classical molecular dynamics were checked against experimental data to make sure they were reliable for the calculations used in this project.

Reviewer 3:

The reviewer indicated the approach followed the project goal of Li-ion conduction in electrolyte and coating material toward stable SEI formation.

Reviewer 4:

The reviewer said it seems overall that the approaches are good but expressed skepticism that ab-initio MD can be used to dot model melt-quench processes. The reviewer elaborated that the simple issue is one of time scales, where melt-quenching takes hundreds of milliseconds and ab-initio MD maxes out in the picosecond regime. The reviewer pointed out that this is an 8 order-of-magnitude gap. The reviewer also has the same issues with using first principles (Vienna Ab initio Simulation Package [VASP], for example) to treat electrochemical processes.

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 all technical accomplishments are relevant and stay in line with scheduled milestones. The reviewer also found that results obtained on Li mobility in highly concentrated liquid electrolytes using first principles, semi-empirical molecular dynamics, and static computational approaches is very relevant and useful for designing novel Li-ion rechargeable batteries with low cost, high capacity, energy density, and safety. Also, computational identification of Li-ion conduction mechanisms in silicon-tin (Si-Sn) alloy helps evaluate overall lithiation and de-lithiation processes taking place in the Si-anode during the electrochemical cycling. This reviewer concluded that the work demonstrates very good progress in addressing the key technical barriers of the Li-ion secondary batteries.

Reviewer 2:
The reviewer stated that the project was able to work toward the goal of Li-ion conduction in the electrolyte and coating material toward stable SEI formation.

Reviewer 3:
The reviewer indicated there were very strong technical accomplishments and encouraged the PI to focus some future work on the Si-SEI, which remains at the heart of the cycle, and calendar-life issues with Si-containing cells. The reviewer added that conduction through Si alloys is not a critical issue.

Reviewer 4:
The reviewer remarked that the project made good progress on three problems including Li-ion conduction in non-aqueous, super-concentrated electrolytes; Li-ion conduction and oxygen transport in amorphous oxide coating materials; and Li-ion conduction and phase behavior in Si-alloy anodes. The reviewer added that while significant progress has been made on all three problems, for the super-concentrated electrolytes, the calculation has not found a real difference in the ion-conduction mechanism and yet no modifications to the electrolyte have been proposed.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the project involves excellent collaboration and coordination on the teams involved in the work such as the Sn-Si alloys.

Reviewer 2:
The reviewer said the project team has been collaborating with LBNL and University of Rhode Island and such a collaboration seems very fruitful.

Reviewer 3:
The reviewer found that it appears the PI was able to work successfully with the National Renewable Energy Laboratory (NREL), LBNL, and a university partner.

Reviewer 4:
The reviewer said there was very good collaboration, but perhaps the PI could include collaboration with experimental teams doing work on oxide coatings on NMC 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 the future direction is clear and relevant. The reviewer stated that additional work will provide more insight into the ionic-diffusion mechanisms taking place in various amorphous oxides as well as Si-based anode materials, which is needed for better understanding of the transport phenomena during the electrochemical cycling.

Reviewer 2:
The reviewer remarked that due to phase separation of the Si-Sn phase upon lithiation, ternary system work will be beneficial.

Reviewer 3:
The reviewer said this project is 90% finished and the plans for the remaining 6 months seem fine.

Reviewer 4:
The reviewer said good, and added that one recurring issue is the normally non-conformal nature of coatings, which offer just partial protection against high-voltage reactions between the electrolyte and the NMC surface.

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

Reviewer 1:
The reviewer agreed that the project is highly relevant and directly supports the DOE overall objectives, adding that design of Li-ion batteries with low price, high energy density, and excellent cyclability is the main VTO program objective and the present project significantly contributes into achieving this challenging goal.

Reviewer 2:
The reviewer stated it was highly relevant with very good focus.

Reviewer 3:
The reviewer said this research will help to understand phenomena going on during lithiation, and that it will help simulate what was obtained for aluminum (Al) and zinc (Zn) systems.

Reviewer 4:
The reviewer indicated that the various problems that are the focus of this work do support the DOE objectives.

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

Reviewer 1:
The reviewer found very good value for the R&D funding investment.

Reviewer 2:
The reviewer stated that the project team has sufficient financial, computational, and human resources to complete the project in a timely manner.

Reviewer 3:
The reviewer suggested that looking toward automotive research, e.g., with GM and small startup doing similar research, may be beneficial if data sharing can work

Reviewer 4:

The reviewer said the resources are sufficient.

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 six reviewers evaluated this project.

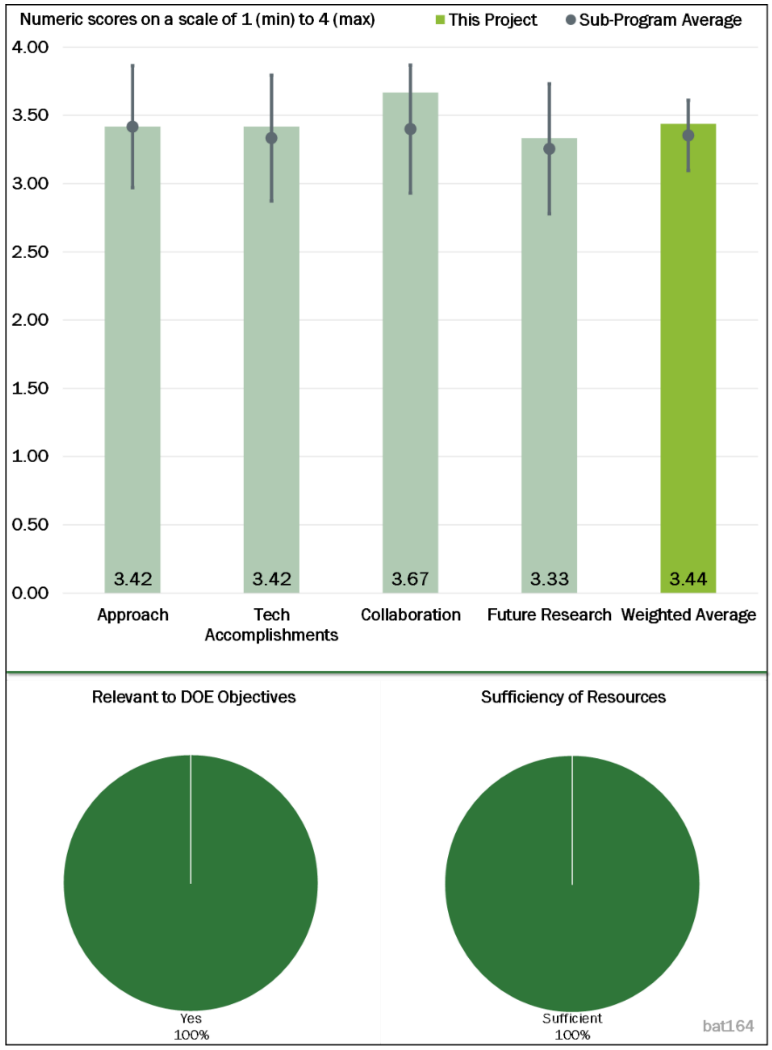

Figure 2-6 – Presentation Number: bat164 Presentation Title: Thick, Low-Cost, High-Power Lithium-Ion Electrodes via Aqueous Processing Principal Investigator: Jianlin Li (Oak Ridge National Laboratory)

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 stated that the approach is well defined and strictly followed, resulting in impressive progress. The reviewer noted that industry has been working on developing water-based electrode production processes for some time, with not much progress on the cathode side, adding that that a well-known company practicing water-based processing is Leclanché. The reviewer suggested that the team might want to reach out and benchmark their results. In general, the reviewer said, high-Ni chemistry is sensitive to moisture; thus, the electrochemical results demonstrated are very intriguing and promising.

Reviewer 2:

The reviewer said the project is well designed and the technical approach with the aqueous processing of thick cathode to address electrode cracking and mass transport limitation led to low processing cost cathode with similar performance as compared to that of a cathode with the N-Methyl-2-pyrrolidone (NMP) method.

Reviewer 3:

The reviewer stated the approach seems good.

Reviewer 4:

The reviewer explained that the approach in this project involves utilization of aqueous processing for Li-ion battery electrode fabrication with the goal to reduce battery pack cost and simultaneously improve cell energy and power density. The reviewer elaborated that achieving this goal also requires fabrication of thick electrodes and utilization of high-voltage cathode materials. Specifically, in the reviewed project period, the team explored this approach to fabricate Ni-rich NMC-811 electrodes. The reviewer added that performance of the electrodes fabricated using aqueous processing is compared to that of the electrodes fabricated using standard NMP solvent. The reviewer pointed out that an interesting aspect of the approach is characterization of the electrolyte imbibition rate, which is particularly important for thick electrodes. The reviewer also noted that a variety of electrochemical characterization techniques were used including cycle life, rate capability and 1,000 USABC 0.33 coulomb (C)/-0.33 C cycles, area-specific impedance of the cells, cycling at different temperatures, and cycling of the thick electrodes with increasing thickness.

Reviewer 5:

The reviewer remarked that aqueous processing will lower costs and be more environmentally friendly—a good target for the project. The reviewer was glad some aspect of making thick electrodes work from a mass transport perspective is included in this project (laser process); however, no results for that were shown. The reviewer suggested that more performance metrics need to be obtained for the aqueous coated materials—gassing, resistance growth on storage, low temperature, etc. This is rather a dramatic change for high-Ni materials, the reviewer said, so evaluation needs to be very thorough. Also, the reviewer noted that the times and scales for slurry mixing and coating that are used in manufacturing should be replicated here.

Reviewer 6:

While noting that the approach seems reasonable, it was not clear to the reviewer what type of binders are being investigated that allowed for aqueous processing versus NMP solvent-based processing. The pH of dispersion, rheological properties, and stability of slurries were also not clear to the reviewer, who added that one would expect different type of functional groups on oxide materials when processed through aqueous solvent versus NMP. It is important to note whether or not the cathode materials used are coated.

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 there were excellent results based on pilot production, adding it was an interesting new methodology to characterize electrolyte imbibition through modeling. The reviewer added that there was good progress on understanding differences in slurry additives in water versus NMP. The reviewer concluded that it is important to conduct X-ray diffraction (XRD) studies and Rietveld analyses to monitor structural changes, if any, in cathode materials exposed to water and processed in water as well as measure alkalinity (free Li content).

Reviewer 2:

The reviewer indicated that cost reduction with the proposed aqueous processing of the cathode has not been provided. The reviewer elaborated that the issue is that the aqueous process cell (NMC-811 cathode) capacity at 1,000 cycles is about 5% less than that with NMP-based process. The reviewer said it would be interesting if a cost analysis can be made to see if it is cost effective for a battery pack based on battery lifecycle for different cathode processing techniques, adding that it is unclear if there is any plan for patent licensing to commercial customers.

Reviewer 3:

The reviewer said the accomplishment and progress seem good but was unsure why there is a need for laser-structured electrodes.

Reviewer 4:

The reviewer explained the four technical accomplishments and progress: First, aqueous processing was applied to fabricate NMC-811 cathodes; it was found that capacity retention in 1,000 USABC 0.33C/-0.33C cycles test of the aqueous-processed electrodes is 70% as compared to 76% in case of NMP-processed electrodes. Second, three different binders compatible with the aqueous processing are characterized using various electrochemical testing techniques. These include: (a) 1 wt. % CMC with 4 wt. % Solvay Latex Emulsion; (b) 1 wt. % CMC with 4 wt. % JSR TRD202A Emulsion; and (c) 5 wt. % Li polyacrylate (LiPAA).

Third, area specific impedance (ASI) of the cells with aqueous-processed electrodes is characterized throughout 100 cycles. The ASI of NMP-processed electrodes is the lowest; however, the difference between this and ASIs of the aqueous-processed electrodes is not dramatically large. The ASI increases with temperature. Fourth, the electrolyte imbibition study is particularly important for thick electrodes. It was found that electrolyte imbibition reduces with lower porosity and higher salt concentration. The activation energy in electrolyte imbibition was determined for the first time. This study provides guidance in electrolyte formulation and electrode engineering.

The reviewer then offered the following observations and suggestions. First, one of the objectives of this project is to optimize electrode fabrication parameters for the aqueous-processed electrodes. However, the presented results only showed results with different binders, for slurry mixing at different temperatures, and for thick electrodes of three different thicknesses only. It is desirable to optimize other parameters of the electrodes fabrication, such as for example (1) water-to-solid mixture (active material, conductive carbon additive, and binder) ratio; (2) ratio of the components in the solid mixture to active material to conductive carbon additive to binder; (3) size of the particles of the active material; (4) nature of the conductive carbon additive and the role of carbon surface functionalization; (5) time of mixing at various stages of the electrode fabrication, etc. The reviewer said that the performance of the aqueous-processed electrodes can be further improved by optimizing these and other electrode fabrication parameters. It is also important to note that these parameters need to be optimized for each electrode material individually.

Second, more detailed surface characterization for the active materials is desired. Although no structural or chemical changes were observed for the 8-10 micrometer (µm) large active materials particles, this could be happening due to the large particle size. Some previous reports showed distinct surface changes of layered transition metal oxide cathodes during exposure to aqueous environments. While these effects could be negligible in the case of large active material particles, they still can contribute to the performance decay. The reviewer encouraged the project team to look into surface changes using approaches such as XPS more closely, as their conclusion that capacity fade could be due to electrode formulation, slurry preparation, and water exposure is too vague. Better understanding of these aspects is desired. The reviewer said it could explain higher ASIs of the aqueous-processed electrodes, especially at elevated temperatures. Third, the reviewer remarked that it is highly desirable to see performance of the cells with aqueous-processed electrodes at high current rates, which is necessary to evaluate the potential of the aqueous-electrode processing for batteries with fast-charging capability.

Reviewer 5:

So far, the reviewer commented, the accomplishment seems to be technologically important and on target, adding that it is important to accomplish more scientific understanding on switching binders and solvents.

The reviewer asserted that techno-economic analysis had not been done to understand the benefits of aqueous processing versus NMP processing in terms of cost savings and wondered how much of this process will allow for reduction in battery cost in dollars per kilowatt-hour.

Reviewer 6:

The reviewer remarked that the project has made progress in demonstrating performance of aqueous-processed electrodes, but more performance metrics are necessary. The reviewer would like to ensure that the NMP baseline is a fair comparison, noting that the performance of NMC-811 is very sensitive to binder, conductive carbon, electrolyte, and anode. The reviewer suggested making the performance using NMP processing as good as it can be, and then comparing that with the aqueous processing, adding that these cells need to be cycled longer.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer affirmed the presence of an excellent combination of industrial and academic partners, adding that it was good to have seen the project team getting feedback and input from battery manufacturers.

Reviewer 2:
The reviewer pointed out that the main team of researchers is located at Oak Ridge National Laboratory (ORNL) and uniquely has access to the pilot-scale electrode processing and pouch cell evaluation battery manufacturing R&D facility. In addition, the reviewer noted, the team benefits from multiple collaborations with the top institutions and companies involved in battery research and development. The reviewer concluded that such a strong team and partners are uniquely positioned to obtain results that would be otherwise impossible.

Reviewer 3:
The reviewer praised the collaboration and coordination across project team as excellent. The reviewer referenced prior comments, and said that some members should focus more on fundamental studies to understand the rheology of slurries and different types of binders that could be used and the drying effect.

Reviewer 4:
The reviewer stated that the team consists of academia and industry partners and added that the team members have a good collaboration.

Reviewer 5:
The reviewer said there is good collaboration between National Laboratories and industry.

Reviewer 6:
The reviewer commented it is a commendable fact that the team is already working with equipment manufacturers and potential end users.

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 the future research in this period (remainder of the year 2019) will be focused on fabrication and performance characterization of the laser-structured electrodes and achieving target performance characteristics (for example, energy density ≥225 Wh/kg on the cell level). The reviewer elaborated that in the following year, the team aims at exploring freeze-tape cast, Ni-rich NMC cathodes, optimizing tortuosity in the electrode architecture, fabricating denser electrodes, and evaluating electrochemical performance of the fabricated electrodes. The reviewer also added that it is highly desirable to see electrochemical performance at high current rates and better understand surface modification of the active materials during aqueous processing of the electrodes.

Reviewer 2:
The reviewer offered that the proposed future research is adequate, although battery research (with the aqueous process) cost-saving analysis for the long-term life cycle is missing from the future plan, adding that cost savings is certainly one of the keys to attract customers.

Reviewer 3:
As mentioned by previous reviewers, this reviewer said, it is important to provide cost analyses, including treatment of the waste streams resulting from this process, adding that it is also important to demonstrate mechanical integrity of the water-processed electrodes.

Reviewer 4:
The reviewer commented that future work seems straight forward.

Reviewer 5:
The reviewer said the proposed future work seems fine. The reviewer commented that it seems like a long project period, 2014-2022, or 8 years. The reviewer asked if that correct.

Reviewer 6:
The reviewer remarked that more work needs to be done to get thicker electrodes, and this project seeks to do that. The reviewer suggested the project team make sure the solution is robust and to test its aqueous process with several high-Ni cathode materials. The reviewer commented that it would be unfortunate if a solution were found for one material, but the process needed to be started over for a new one.

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

Reviewer 1:
The reviewer agreed that this project supports DOE objectives by addressing battery-production cost reduction and energy-density increase with thick electrodes.

Reviewer 2:
The reviewer affirmed that this project supports the overall DOE objective by investigating several aspects of batteries, adding that it was nice to have seen two patents filed.

Reviewer 3:
The reviewer remarked that this research is relevant to the DOE efforts in developing safer, low-cost Li-ion batteries with high-energy density and high-power density. The reviewer mentioned that cost reduction is intended to be achieved via replacing expensive NMP-based electrode processing with aqueous processing, adding that in addition to the cost reduction, aqueous processing is safer than that involving NMP.

Reviewer 4:
Yes, the reviewer agreed, the manufacture of thicker electrodes (that perform well) with aqueous processing will ultimately lower battery costs. The reviewer remarked that a lower cost of the batteries can help enable widespread adoption of EVs, which is specifically a DOE objective.

Reviewer 5:
The reviewer stated that aqueous processing of battery electrodes can help reduce the costs and hazardous nature of working with organic solvents.

Reviewer 6:
The reviewer said yes, adding that the project is focused on cost reduction and environmentally friendly industrial processes.

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 available for the team are highly adequate.

Reviewer 2:
The reviewer found a right mix of collaborators and partners.

Reviewer 3:
The reviewer commented that the team has the necessary equipment and capabilities to do this project, especially with input and feedback from partners.

Reviewer 4:
The reviewer said the budget and resources used are appropriate.

Reviewer 5:
The reviewer stated that the resources seem sufficient.

Reviewer 6:
The reviewer remarked that the resources appear to be sufficient to support the proposed research.

Presentation Number: bat183
Presentation Title: In-situ Spectroscopy of Solvothermal Synthesis of Next-Generation Cathode Materials
Principal Investigator: Feng Wang (Brookhaven National Laboratory)

Presenter

Feng Wang, Brookhaven National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

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

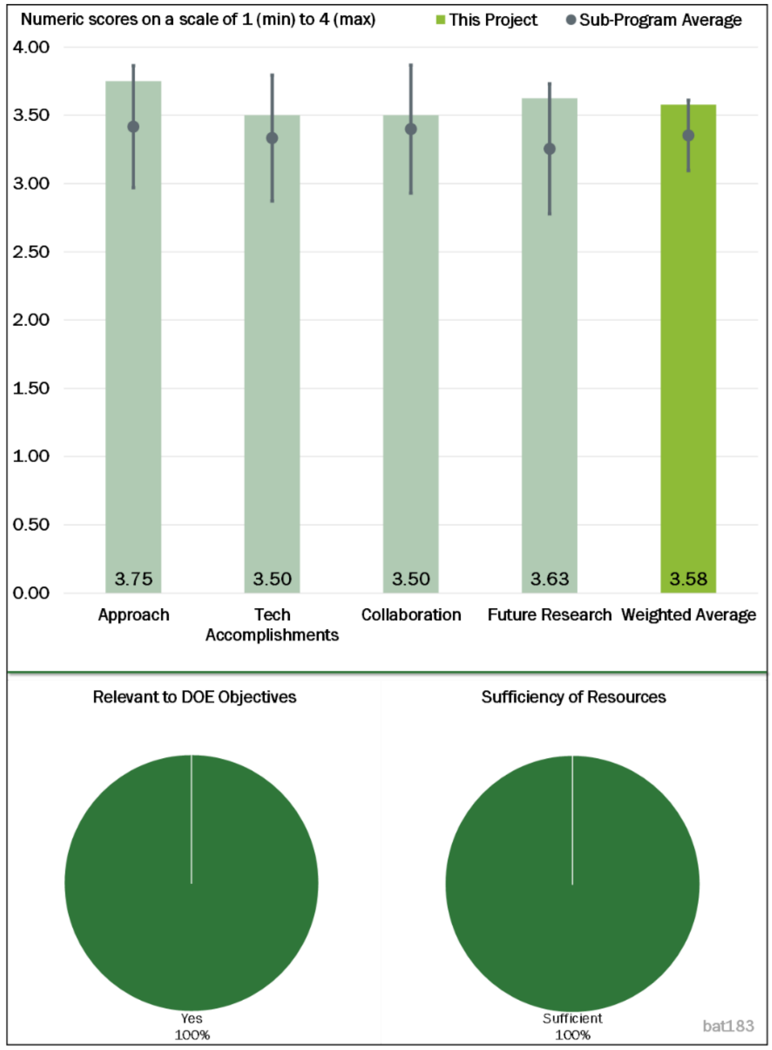

Figure 2-7 – Presentation Number: bat183 Presentation Title: In-situ Spectroscopy of Solvothermal Synthesis of Next-Generation Cathode Materials Principal Investigator: Feng Wang (Brookhaven National Laboratory)

Reviewer 1:

The reviewer praised the great technique, adding that this has a lot of potential to reduce cost and improve performance. The reviewer pointed out that cost and performance depend upon both composition and synthesis and this technique can help understand the variable space. The reviewer did not know the rate that experiments can be performed but would push for some nice statistical design of experiments involving composition and process. The reviewer declared that there is the potential for good outcomes here.

Reviewer 2:

The reviewer stated that in situ studies of NMC materials synthesis are very important, adding that they can yield very important information about compositional uniformity and phase purity and also allow us to understand the evolution through nucleation and growth during the process. The reviewer also noted that the project includes several in situ techniques specifically with X-ray diffraction and absorption.

Reviewer 3:

Today, the reviewer said, there are not many cathode producers that could produce high-quality, high-Ni materials. The reviewer asserted that the approach is very novel and potentially can have a very positive impact on commercialization of these materials. Surprisingly, the reviewer added, the initial results already support ex situ studies and theories.

Reviewer 4:

The reviewer offered that the approach seems like a unique approach and that it might be interesting if the project team could determine local strain and depth-of-transition metal (TM) dissociation. The reviewer added that density functional theory (DFT) modeling might be able to help here.

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 was looking forward to the outcome of the theoretical and in-situ synthetic results, adding that these should be extremely valuable for the industry. The reviewer concluded that the work to date shows high probability of success.

Reviewer 2:

The reviewer suggested the team take a more systematic approach to studying the variable space. Use statistical design, the reviewer commented, as this setup is perfect for that.

Reviewer 3:

The reviewer remarked that in situ techniques are yielding great deal of information about composition evolution, ordering, and Li deficiency. The reviewer's only recommendation is to study early-stage studies to understand alloy formation and the corresponding nucleation and growth aspects and to consider as what the motivating factors are that drive phase formation and their relationship to the process conditions. The reviewer added it would also be very interesting to study such synthesis under conditions that are quite different from those typically used.

Reviewer 4:

The reviewer said that technical accomplishments seemed good, adding that the transition-metal dissolution research was interesting. The reviewer also said it would have been interesting to see theoretical DFT predictions to confirm findings.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that collaboration and coordination among the team is excellent.

Reviewer 2:

The reviewer found good collaboration with DOE Laboratories.

Reviewer 3:

The reviewer did not see any issues here, but wondered where industry is. The reviewer recommended getting some input from outside the working team to figure out what is commercially relevant.

Reviewer 4:

The reviewer said that while the presentation was a little bit confusing, project team members tried to compensate by clarifying and explaining certain points, a fact that demonstrates true team spirit.

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 future work seems good and to keep going.

Reviewer 2:
The reviewer remarked there was good understanding of what needs to be done and how as well as where results could be applied. The reviewer will be following up on progress.

Reviewer 3:
The reviewer recommended including more experiments on cost reduction, as in reduction in energy consumption, lower cost precursors, less excess Li source, etc. The reviewer thought this would be a very valuable outcome of this project.

Reviewer 4:
The reviewer found that the proposed studies seem to be rational and logical. As mentioned before, early-stage studies combined with non-typical synthesis conditions could yield some interesting information.

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

Reviewer 1:
The reviewer stated that this project supports the DOE objective by further improving battery technology.

Reviewer 2:
The reviewer offered that finding lower cost synthesis methods or better compositions for high-energy cathodes will enable battery technology that meets DOE vehicle targets, adding that this project can do both.

Reviewer 3:
The reviewer commented that NMC materials and their synthesis are very important to DOE's mission. The reviewer added that fundamental insight into their synthesis is very important for advancing battery research.

Reviewer 4:
Ultimately, the reviewer remarked, understanding and controlling of the synthesis parameters will lead to the increased availability of high-energy density materials at reduced 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 found a highly motivated team.

Reviewer 2:
The reviewer stated the resources seemed good.

Reviewer 3:
The reviewer said the resources are adequate.

Reviewer 4:
The reviewer said that resources seem okay. If possible, the project team should get more experiments done in the timeframe it has.

Presentation Number: bat207
Presentation Title: Toward Solventless Processing of Thick Electron-Beam (EB) Cured Lithium-Ion Battery Cathodes
Principal Investigator: David Wood (Oak Ridge National Laboratory)

Presenter

David Wood, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

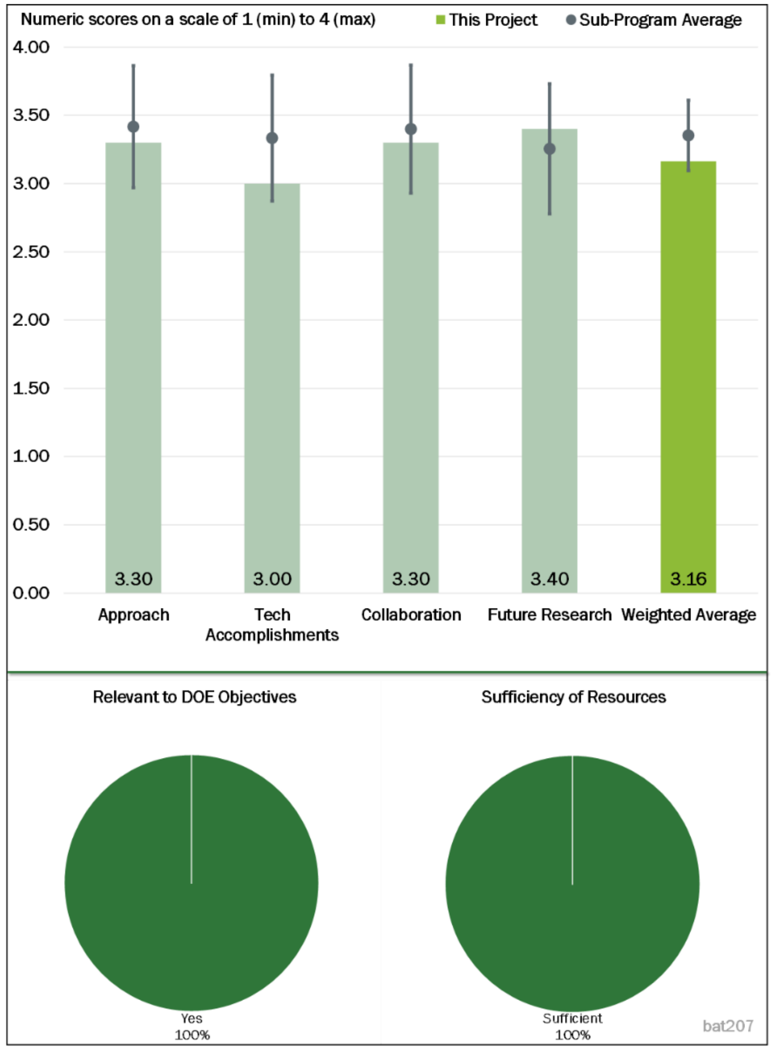

Figure 2-8 – Presentation Number: bat207 Presentation Title: Toward Solventless Processing of Thick Electron-Beam (EB) Cured Lithium-Ion Battery Cathodes Principal Investigator: David Wood (Oak Ridge National Laboratory)

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 stated that the technical approach sounds productive to address production-cost savings and production-speed increase.

Reviewer 2:

The reviewer explained that the approach in this project is based on developing solvent-free processing of electrodes, including thick electrodes, using electron-beam (EB) curing for fabrication of Li-ion battery cathodes. The reviewer elaborated that in this approach a liquid binder is used, which is dried by EB curing. This approach can reduce the cost and increase energy efficiency of the battery manufacturing process. In addition, the reviewer said, this electrode-processing technology requires equipment that takes less space than conventional drying ovens used in the currently established electrode-processing procedures. Moreover, the reviewer added, EB-assisted electrode fabrication is a high-speed process that can enable rapid battery manufacturing.

Reviewer 3:

The reviewer stated that the suggested approach is good and much different from that being practiced in the industry right now. The reviewer stated that the approach is okay to demonstrate the validity of the technique.

Reviewer 4:

The reviewer commented that while the approach to make thick electrodes without solvent is a good idea, it really does need to get coupled with efforts to move electrolyte within those thick electrodes. The reviewer suggested that this project needs a good cost assessment. Pointing out that current electrode loadings of 4-5 mAh/cm^2 can be made using traditional methods, the reviewer noted that this project targets 6-8 mAh/cm^2, and asked if the cost/benefit ratio is worthwhile.

Reviewer 5:

The reviewer said the approach using EB seems like a unique approach and interesting. The reviewer is surprised there is not significant damage to the material, and asked what about microwave curing?

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 cells made with the solventless-processed thick cathode seems have a good performance with limited cycle testing.

Reviewer 2:

The reviewer commented that progress seems good so far but added that it might be worthwhile to look at material post-dose in a scanning electron microscope (SEM).

Reviewer 3:

The reviewer explained that the project is currently in its third phase, in which the goal is to demonstrate ultra-thick cathode coatings and an optimized curing system in conjunction with a high-speed coating line together with a key equipment partner and battery manufacturer. The reviewer made three points. First, high speed EB-curing of NMC-622 and NMC-811 electrodes has been demonstrated. The presence of oxygen during electrode fabrication was identified as an issue, and a molecular nitrogen (N_2) blanket needs to be used to enable efficient binder crosslinking. Reducing oxygen content leads to higher capacity and lower polarization in electrodes. Second, aa new EB-curable resin for NMC-622 cathode with a Keyland polymer was developed and demonstrated cell capacity and capacity retention similar to PVDF. Third, an electrostatic spraying process was developed to demonstrate good adhesion of the electrode film to the current collector and uniform electrode-film thickness.

The reviewer asked for more information and made suggestions regarding the following: First, given the delay in delivering a piece of equipment for the roll-to-roll, EB-curing electrode-manufacturing process, the reviewer inquired how the project will be modified to guarantee timely implementation. Second, with the results demonstrated at this review meeting, it is necessary to provide electrochemical testing results, which should include multiple electrochemical techniques. For example, the reviewer wanted to know how the electrodes fabricated using the proposed processing method perform at high currents. Resistivity of the electrodes need to be characterized, together with the standard cycle-life and rate-capability experiments. Electrolyte imbibition, demonstrated ORNL researchers, and characterization should also be provided, especially for the thick electrodes.

Reviewer 4:

The reviewer noted that this project started in 2015, but progress seems to be limited by using equipment at vendors or other locations. The reviewer thought progress will accelerate when the equipment is set up at ORNL. The reviewer also noted that the pouch cell go/no-go decision in 2018 has been delayed until the third quarter of 2019, indicating the project is a bit behind.

Reviewer 5:

The reviewer observed that the technical accomplishments demonstrate validity of the technique. The reviewer suggested that the techno-economic analysis should be done to see on how much this technique could reduce the overall costs of energy storage. Stating that such cost analysis should be done, the reviewer added that the experimental plan should include pre-commercial scale trials to elucidate the problems associated with such technology. Otherwise, the reviewer said, the development of such techniques could just become an academic exercise. Also, it was not clear to the reviewer why EB curing is more interesting than UV curing.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer indicated the project had collaboration by both industry partners and a National Laboratory, adding that the collaborations among team members are productive.

Reviewer 2:

The reviewer commented that the project has industry involved, which is good, adding that the team includes a resin supplier, equipment suppliers, and battery companies. The reviewer remarked that this sets a good example for DOE-funded projects.

Reviewer 3:

The team is based at ORNL, the reviewer said, but noted that it works with multiple industry partners.

Reviewer 4:

The reviewer remarked the collaboration with industrial partners is very good but added that the exact role of battery manufacturers in this project is unclear.

Reviewer 5:

The reviewer said that collaboration seems good, but that it was difficult to determine what everyone's contributions were.

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

Reviewer 1:

The reviewer explained that electrochemical performance of the cells with EB-cured electrodes will be evaluated. An important step to be done in the near future is the installation of a roll-to-roll, EB-curing pilot line at ORNL. The reviewer elaborated that electrostatic spraying process with EB curing for thick electrode fabrication will be developed for NMC-811 electrodes and that further resin development is planned.

Reviewer 2:

The reviewer stated that the proposed future research is sound but suggested having lifecycle testing of cells with developed cathode solventless processing in order to prove the developed technique is effective for cell lifecycle cost saving.

Reviewer 3:

Stating that the future work sounds good, the reviewer suggested some SEM images just to see what is going on.

Reviewer 4:

This reviewer commented that the project needs to get equipment set up and generate results—those are the next steps. The reviewer remarked that the investigators need to evaluate the robustness of the approach with different cathode materials, loadings, anode materials, particle size, etc. The reviewer said it would be a disappointment to do all development on a limited material set and to have to start all over again with a new material.

Reviewer 5:

The reviewer stated that the future research seems straightforward and added that it is not clear what the technical targets are that need to be met prior to battery manufacturers' acceptance of this technique. The reviewer said that such target specs would be good to establish.

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

Reviewer 1:
The reviewer found great relevance to advancing battery technology.

Reviewer 2:
The reviewer agreed that the project supports DOE's objective on battery-cost reduction and energy-density increase.

Reviewer 3:
Offering that finding lower cost manufacturing methods or better compositions for high-energy cathodes will enable battery technology that meets DOE vehicle targets, the reviewer stated that this project can do both.

Reviewer 4:
The reviewer stated that the research is relevant to the DOE efforts in developing energy-efficient and low-cost processes for high-energy and high-power Li-ion batteries manufacturing. The reviewer explained that energy efficiency and cost reduction are intended to be achieved via replacing expensive NMP-based electrode processing with EB treatment, a fast and robust materials-processing technology. Additionally, the reviewer said, such technology can enable desirable ultra-high electrode processing speed.

Reviewer 5:
The reviewer stated that this project provides an alternate method of coating without using any solvents. The reviewer added that this will contribute to modernizing the electrode coating and battery-making process and will potentially lower the cost of manufacturing.

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 funding assigned to this project seems adequate for the proposed work.

Reviewer 2:
The reviewer stated that resources are sufficient.

Reviewer 3:
The reviewer said that resources seem fine. The reviewer is sure the project team can find a SEM machine to take some images.

Reviewer 4:
The reviewer stated the majority of resources available for the team are adequate but added that the installation of the roll-to-roll EB-curing pilot line at ORNL that caused delay in achieving progress in this project is critical.

Reviewer 5:
The reviewer said the resources seem okay, but if possible, suggested the project team get more experiments done in the timeframe it has. The reviewer added that having in-house coating equipment will help here.

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

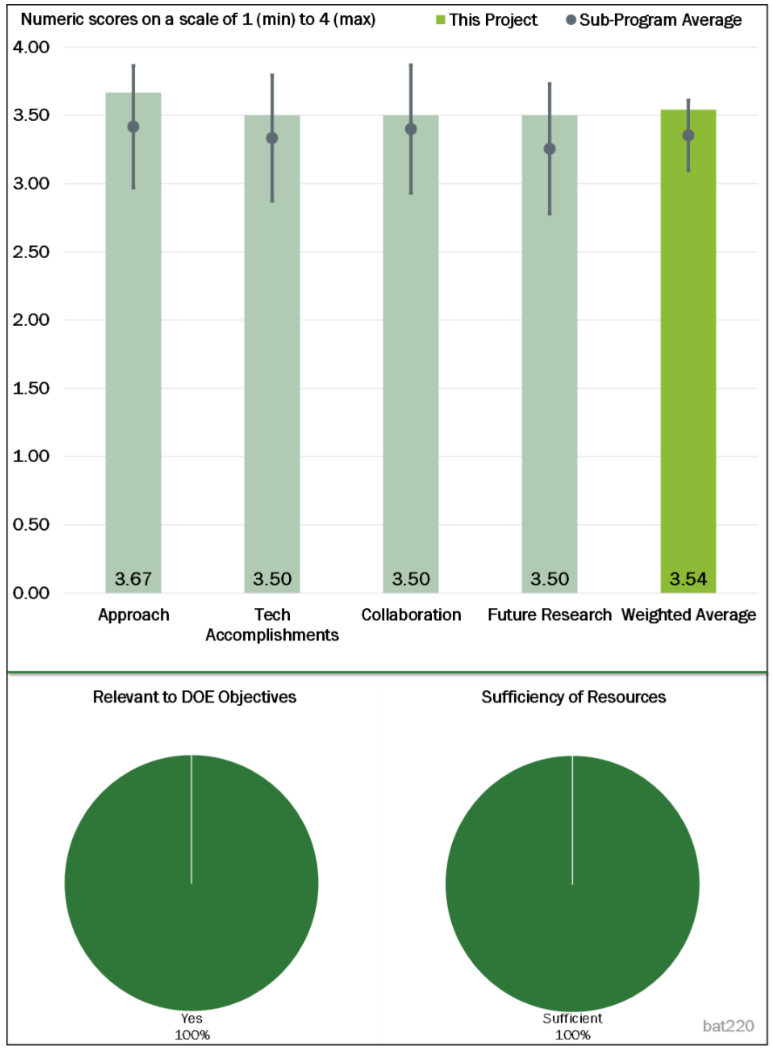

Figure 2-9 – Presentation Number: bat220 Presentation Title: Addressing Heterogeneity in Electrode Fabrication Processes Principal Investigator: Dean Wheeler (Brigham Young University)

Presenter

Dean Wheeler, 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 explained that this project has developed a range of experimental and modeling tools to measure and predict localized properties. The reviewer elaborated that the developed flexible micro-line probe is well designed to perform localized conductivity measurements on lithium-iron phosphate (LFP) cathode films. The reviewer also stated that the smoothed-particle hydrodynamics model provides precise prediction of porosity validated with the experimental results. The constructed laser-based acoustic probe is technically sound to estimate the Young’s modulus of the battery coating. Overall, the reviewer said, the proposed approach can well address the technical barriers.

Reviewer 2:

Noting that the heterogeneity of electrodes in fabrication results in a short life of batteries, the reviewer explained that the team explored approaches to probing the ionic and electronic conductivities of various electrodes. The reviewer stated that these approaches seem effective and might be used in production.

Reviewer 3:

The reviewer said that the research work has been well performing with good achievement, adding that the technical barriers were clearly determined for each stage and the team effectively came up with possible and comprehensive solutions.

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 deliverables of flexible probes for conductivity measurement, acoustic probe for mechanical properties, and demonstrated industrial partners have been properly achieved according to the project progress. The reviewer also said that milestones have been met and the technical accomplishments made in the project are satisfactory.

Reviewer 2:

The reviewer said the electronic conductivity probe developed in this project has been sold to a third party and that various electrodes have been tested.

Reviewer 3:

The reviewer observed that the milestone in Year 2 has been well on track and effectively planned to continuously improve the first-stage commercial conductivity probe.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer observed that the research group has a wide collaboration with different partners (from different institutions) for exchanging battery materials and expertise in this field.

Reviewer 2:

The reviewer noted that a lot of collaborators supplied samples but added that it is better to have a company that is interested in commercializing the devices.

Reviewer 3:

The reviewer commented that the project team has non-contractual partnerships and collaborations with multiple industrial partners, academic universities, and National Laboratories. However, the reviewer added, the project has not shown the measurement results for some materials supplied by several partners such as EaglePicher and Utah State 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 commented that the project has a good plan by clearly determining the goal and considering barriers to the realization of the outstanding technology.

Reviewer 2:

The reviewer stated that proposed activities can effectively close this project.

Reviewer 3:

The reviewer remarked that proposed future research on creating a design package for commercialization of conductivity probes and modeling are effectively planned. However, the reviewer added, the project has not clarified the future research plan on acoustic probes to localized mapping of film stiffness even though this is one of remaining challenges and barriers.

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

Reviewer 1:

Reviewer 2:
As clearly stated, the reviewer indicated that the project's objectives fall into the DOE VTO mission. The reviewer elaborated that this work addresses a longstanding unmet industry need to be able to conveniently measure physical properties of thin-film electrodes and detect manufacturing variations and changes during cycling—solving this problem will accelerate process improvement, reduce scrap rates, and lower battery costs. This reviewer added that the work will improve Li-ion battery technology in EVs and at the grid scale, which will reduce energy costs to businesses and consumers, increase energy security, and allow clean energy technology to move people and goods.

Reviewer 3:
The reviewer said that the project fully supports the DOE objectives for elucidating connections between fabrication conditions and undesired heterogeneity of thin-film electrodes by non-destructive inspection techniques and computer models.

Reviewer 4:
The reviewer explained that this project aims to understand the fabrication conditions and undesired heterogeneity of battery electrodes, which potentially help manufacture better batteries.

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

Reviewer 1:
The reviewer stated that the resources for the project are sufficient to achieve the milestones timely.

Reviewer 2:

Reviewer 3:
The reviewer said that resources are enough to cover the milestones of the project in a timely fashion, explaining that milestones for this project end in September 2019 but work will continue until December 2019 due to an initial delay in the contract.

Reviewer 4:
The reviewer had no comment.

Presentation Number: bat225
Presentation Title: Model System Diagnostics for High-Energy Cathode Development
Principal Investigator: Guoying Chen (Lawrence Berkeley National Laboratory)

Presenter

Guoying Chen, Lawrence Berkeley National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

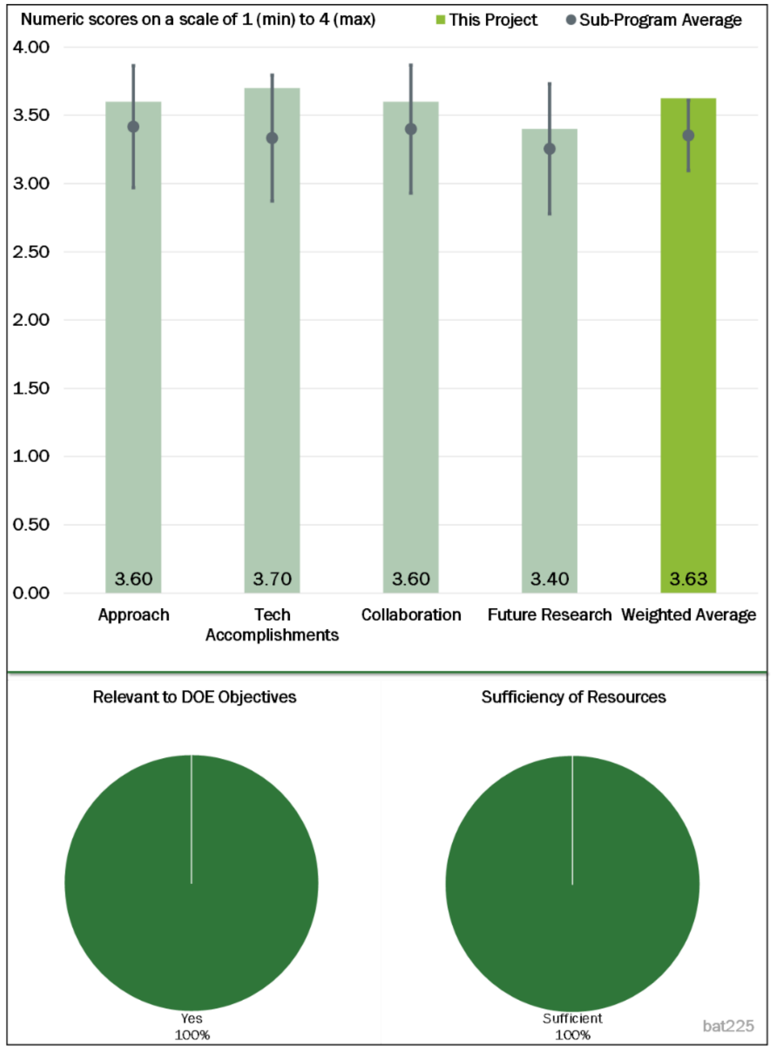

Figure 2-10 – Presentation Number: bat225 Presentation Title: Model System Diagnostics for High-Energy Cathode Development Principal Investigator: Guoying Chen (Lawrence Berkeley National Laboratory)

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 explained that the approach is to use model systems to understand decouple and understand the anion and cation redox chemistry in high-voltage cathode materials using advanced diagnostic techniques. The reviewer said the approach was well developed and the work done was of high quality.

Reviewer 2:

The reviewer wrote that the synthesis of model material is crucial to simplifying, to a certain degree, the complicated electrochemical system that advanced diagnostics needs to uncover hidden knowledge. The reviewer concluded that a comprehensive understanding of electrochemical and interfacial properties of Li-rich cathodes has been demonstrated.

Reviewer 3:

The reviewer stated that an advanced diagnostic technique used by the project team for fundamental understanding of solid-state chemistry, kinetic barriers, and instabilities of high-capacity cathode during battery operation is well designed. The reviewer added that this study is really important for the fundamental correlation of capacity and stability with TM and oxygen (O_2) redox processes, which will help to further develop rational design for next-generation high-energy cathode materials.

Reviewer 4:

The reviewer explained that advanced X-ray-based, neutron-based techniques, and in-operando differential electrochemical mass spectroscopy are combined with electrochemical tests to study the cation redox and anion redox activities in cation-disordered rock-salt, Li-rich cathode materials as a model system. The reviewer elaborated that resonant inelastic X-ray scattering mapping is a very powerful tool to probe the oxygen redox in Li-rich cathode materials. Doping of redox-inactive transition metal is used to suppress irreversible oxygen loss, which is a good and effective method.

Reviewer 5:

The reviewer commented that the work addresses the cycling stability and capacity of cathode materials involving oxygen redox, adding that understanding the mechanisms is important in developing next-generation materials. The reviewer also remarked that the use of a high-quality single crystal helps to define the material and provides more reliable observations than polycrystalline 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 affirmed that excellent progress has been accomplished in this project by using advanced characterization techniques. The reviewer explained that by using synchrotron-based resonant inelastic X-ray scattering and electrochemical testing, the project team concluded that with more and more O_2 redox contribution, the cycling capacity is increased while capacity retention is decreased. The reviewer further explained that by doping redox-inactive transition metal, the PI pointed out that titanium (Ti) is better than niobium (Nb) in suppressing O_2 release and manganese (Mn) reduction in cation-disorder Li-rich cathode materials. Doping with redox-inactive elements can be an important bulk strategy for not only Li-rich cathode materials but also Ni-rich cathode materials. The reviewer concluded progress is good and the milestones are on schedule.

Reviewer 2:

In this budget period, the reviewer remarked that significant work has been performed by the project team. The reviewer elaborated that the project team used advanced diagnostic techniques to identify O_2 loss and the chemical stability effect of a Li-rich transition metal (LRTM) model system by introducing different TM using operando differential electrochemical mass spectroscopy and Mn K-edge hard XAS spectra mapping. A correlation of stability with O_2 redox has been developed in Li-rich TM oxide. The capacity and stability correlation are clearly helpful to design high-capacity Li-rich novel materials by introducing redox-inactive Ti.

Reviewer 3:

The reviewer commented that multiple diagnostic techniques have been utilized to understand the redox mechanism and interfacial process of Li-rich oxides, and that the activity is well-planned and executed. To satisfy the reviewer’s curiosity regarding the density data, the reviewer wanted to know whether the carbon dioxide (CO_2) release occurs at a potential below 4V and how the CO_2 is released during the second cycle.

Reviewer 4:

The reviewer explained that the technical accomplishments have been an understanding of a model Li-rich disordered rock salt cathode material, an understanding of the role of the O_2 anion redox, and how doping D^0 transition metals helps to stabilize the O_2 loss. Finding the work to be well developed, the reviewer said it would be interesting to have seen how anion dopants help further stabilize the O_2, as well as doping on the Mn transition metal and increasing the total Li concentration. The reviewer pointed out that Ceder et al. have shown that by increasing the Li concentration, you can get more Li mobility to a certain point. The reviewer said it would be interesting to use the advanced techniques to understand what mechanisms are at play here. Additionally, the reviewer commented, the differential electrochemical mass spectroscopy (DEMS) work that the project team showed has some anomalies on the charge and discharge profile that does not make sense. It looks like at high voltages on discharge, there is a plateau whereas in normal systems, it is not shown. The reviewer asked why this is manifesting and how it will change the results when not present. The reviewer indicated the team claims that Ti^{4+} is better than Nb^{5+} in suppressing molecular O_2 loss. However, with the weird voltage profile, these results might be muddled, and more work is needed to identify this.

Reviewer 5:
The reviewer said that the role of O_2 redox is confirmed and the role of an inactive element in stabilizing the structure and influencing the O_2 redox is elucidated. The surface effect, however, appears to be very difficult to delineate.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted that the team collaborates with a modeling team (LBNL), synchrotron team (LBNL and Stanford Synchrotron Radiation Lightsource [SSRL]), resonant inelastic X-ray scattering (RIXS) team (Advanced Light Source [ALS]), DEMS team (LBNL), scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) team (Pacific Northwest National Laboratory [PNNL]), and a neutron team (ORNL). The reviewer added that the work clearly shows a great collaborative effort.

Reviewer 2:
The reviewer stated that the PI works with a broad range of teams in the program from computational scientists and electrochemists to TEM and beamline scientists.

Reviewer 3:
The reviewer said that the PI has good collaboration with other National Laboratories, companies, and universities, who are key players in this field.

Reviewer 4:
The reviewer found that the team collaborates well with other Advanced BMR teams and that it makes good use of national user facilities.

Reviewer 5:
The reviewer responded that the group at LBNL has an excellent collaboration with National Laboratory and university partners. However, the reviewer added, the role of the university investigator 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 said that the team has a great plan for further understanding the interplay between the anion and cation redox, how to clearly quantify those, and then design systems with optimal compositions.

Reviewer 2:
The reviewer responded that the future work is well rationalized and outlined.

Reviewer 3:
The reviewer remarked that the proposed future work is impressive on a comprehensive understanding of performance-limiting mechanisms and processes in LRTM oxide cathodes; on development of mitigating strategies; and providing the necessary material design to achieve high-capacity cathodes along with stability. The reviewer also stated that the future plan is adequate to cover the next year.

Reviewer 4:
The reviewer stated that surface modification on cation-disorder Li-rich cathode materials is planned and the PI also proposed to develop surface-sensitive techniques to investigate the surface chemistry. The reviewer concluded that the future research proposed in this project sounds very interesting and relevant to current study.

Reviewer 5:
The reviewer remarked that the direction of the proposed work is a natural continuation of the current work, adding that further understanding the role of surface chemistry is indeed critical. The reviewer encouraged the PI to develop research questions that take full advantage of the use of single crystalline materials (e.g., surface of different facets). The reviewer recommended that the PI be more specific about exact plans for understanding the anion- and cation-redox relationship and added that the same concern exists for the role of surface coating.

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

Reviewer 1:
The reviewer affirmed that the work strongly supports the objectives of DOE by comprehensive investigating the potential barriers for high-voltage and high-capacity cathodes for high-energy density Li batteries.

Reviewer 2:
The project is highly relevant to overall DOE objectives, the reviewer said, which is aimed at developing high-energy batteries with lower cost. The reviewer added that the fundamental understating of the synergetic cation- and anion-redox activity in Li-rich cathode material is very much needed.

Reviewer 3:
According to the reviewer, the effort in understanding the degradation mechanism using advanced characterization techniques and developing mitigation strategies of Li-rich TM cathode is vital for the development of the high-capacity cathodes and that this clearly supports DOE objectives.

Reviewer 4:
The reviewer stated that a fundamental understanding of the redox mechanism of high-capacity cathodes is essential for developing the next-generation batteries.

Reviewer 5:
The reviewer remarked that this work clearly shows relevance as it has a high capacity and high theoretical energy density. The reviewer also said the challenge is to maintain stability, and the project team has been able to start to address this. The reviewer commented that the one key component the project team has left out is the loading, elaborating that the team typically has an 80%:20%mixture to make these by solid-state ball milling, but then add another 10%conductive carbon in the electrode formulation. So, this active material loading is not practical for industry. The reviewer asked if there is a pathway moving forward to increasing the electrode loading.

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

Reviewer 1:
The reviewer affirmed that the team has great resources and has shown this by the great work that has been done so far.

Reviewer 2:
The reviewer stated that the PI takes great advantage of the collaborative effort in the program, and that the current progress is consistent with the funding level.

Reviewer 3:
The reviewer remarked that the current resources are sufficient to achieve the project targets.

Reviewer 4:
The reviewer said the PI has adequate resources to conduct the proposed research.

Reviewer 5:

The reviewer replied that the resources are sufficient.

Presentation Number: bat226 Presentation Title: Microscopy Investigation of the Fading Mechanism of Electrode Materials Principal Investigator: Chongmin Wang (Pacific Northwest National Laboratory)

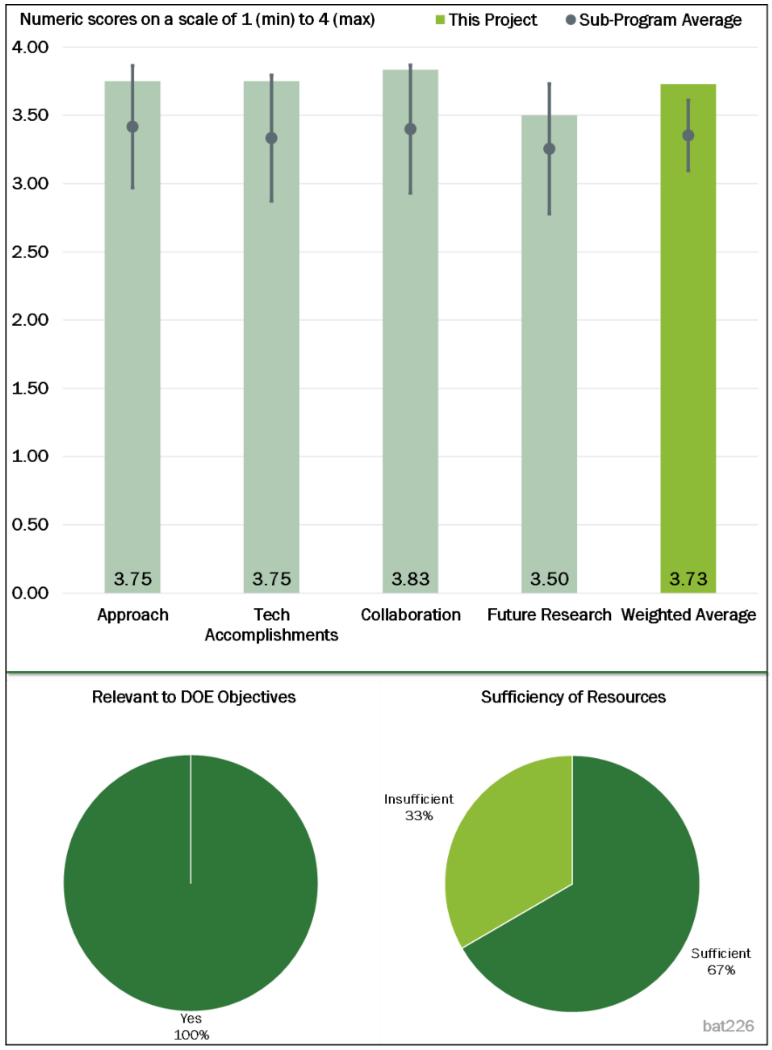

Figure 2-11 – Presentation Number: bat226 Presentation Title: Microscopy Investigation of the Fading Mechanism of Electrode Materials Principal Investigator: Chongmin Wang (Pacific Northwest National Laboratory)

Presenter

Chongmin Wang, Pacific Northwest 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 stated that the PI has been developing powerful in situ TEM and secondary ion mass spectroscopy (SIMS) techniques to understand electrode structure degradation and that these techniques have provided unprecedented insights under dynamic conditions.

Reviewer 2:

The reviewer praised as very comprehensive the approach to diagnosing fading mechanisms in NMC cathode materials, especially given the relatively modest funding level.

Reviewer 3:

The reviewer noted that multiple in situ and ex situ electron microscopy techniques were developed and deployed to understand the structure change of cathode materials during cycling. The reviewer also noted that localized structural change was successfully visualized.

Reviewer 4:

The reviewer explained that advanced electron microscopy techniques, including in situ environmental TEM, STEM-EELS, and three-dimensional (3D) atom probe tomography, are utilized to study the degradation mechanism in Li-rich layered cathode materials and high-Ni-content layered cathode materials. The reviewer found the approach very appropriate for the study, which provides an in-depth understanding of structural and chemical evolution at the atomic level in three dimensions.

Reviewer 5:

The reviewer indicated that spectroscopic techniques (high-resolution transmission electron microscopy [HRTEM], cryo-HRTEM, and SIMS) are effective tools for characterizing battery materials.

Reviewer 6:

The reviewer found that the approach is excellent for atomic-to-nanoscale spatial resolutions, but the major barrier is the poor statistics. The reviewer suggested that the PI should consider showing a way to demonstrate the statistics because the cathode materials have a variety of particles.

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 affirmed that excellent progress has been accomplished in this project by using state-of-the-art electron microscopy techniques. The reviewer explained that the project team has successfully applied the techniques to investigate the O_2 loss and O_2 vacancy migration mechanism in Li-rich layered cathode materials. The reviewer explained that O_2 loss first happens on the surface and then the O_2 vacancy moves from the surface to the bulk material. The results are a very important guide that surface stability is the key point for Li-rich cathode material. In the high-Ni-content system, electrolyte-relevant interface reaction and rate-dependent structure evolution are investigated. The reviewer concluded that progress is impressive and the milestones are on schedule.

Reviewer 2:

The reviewer found very broad and deep accomplishments on O_2 vacancy migration. The reviewer elaborated that it is nice to know that we have to stop surface O_2release, but this O_2 release has been known for a long time and we do not know how to stop it. The reviewer described this work as a very valuable start to understanding the influence that electrolyte chemistry has on surface reactions even with SEI present.

Reviewer 3:

The reviewer remarked that the work on layered Li excess oxide has revealed the new phenomenon of vacancy injection into the bulk as well as how this is correlated with surface and interface chemistry. The reviewer added that this represents a major advancement in the understanding of these materials.

Reviewer 4:

The reviewer concluded there is good progress in 3D tomography, showing void formation at the edge of particles.

Reviewer 5:

The reviewer described as very important the discovery that for a Li-rich layered cathode, O_2 vacancy is gradually injected into the bulk lattice and forms nano-voids that degrade the bulk material.

Reviewer 6:

The reviewer explained that the voltage fade of the Li-rich cathode was attributed to the injection of O_2 vacancies into the bulk of cathode materials during cycling, adding that it was also reported that the control of interfacial reaction can mitigate the bulk lattice degradation. The reviewer indicated that there is no clear explanation on how the chemical environment at the interfacial boundary can be efficiently delivered to the bulk of the materials.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer described very strong collaborations and added that hopefully the team can take these results and formulate novel electrolytes to mitigate fade mechanisms.

Reviewer 2:
The reviewer stated the PI has good collaboration with other National Laboratories, companies, and universities, who are key players in this field.

Reviewer 3:
The reviewer said the team has a good collaboration with industrial and academic partners.

Reviewer 4:
The reviewer remarked that the PI has built an ecosystem that involves other National Laboratories, industry, and equipment makers.

Reviewer 5:
The reviewer commented that the PI is collaborating with many groups including the National Laboratories, universities, and industrial companies.

Reviewer 6:
The reviewer suggested the collaboration team could perhaps have more consistency and the focus will be better. The reviewer added that providing samples alone is not sufficient.

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 it is very nice that the PI is moving to chemistries other than the Li-rich and Mn-rich layered oxides. Also, the reviewer said it is very good that the PI is moving to investigate Li-metal dendrite phenomena and to start using cryo-TEM.

Reviewer 2:
The reviewer indicated that a detailed plan on cathode, as well as the anode interface, has been proposed.

Reviewer 3:
The reviewer explained the PI proposed to investigate the dopant effect and structure defect nature in Ni-based cathode materials. Also, the reviewer said, in situ and cryo-TEM, combined with SIMS, is proposed to be utilized in the study of anode structure and SEI. The reviewer added that the proposed research sounds very interesting and reasonable.

Reviewer 4:
The reviewer remarked that the PI has proposed to extend the techniques to understand the role of Al in NCA. While this is an established material, the reviewer noted that the PI's techniques hold the promise to shed new light on this important material. Over the long term, the reviewer added, the PI has proposed to work on Li-metal, which is also a critical direction.

Reviewer 5:
The reviewer stated that the group will be focusing on some key issues of Li-metal batteries in 2020, and that novel cryo-TEM and EELS investigations will be pursued to obtain detailed structure and chemical information on the Li anode-liquid SEI layer.

Reviewer 6:
The reviewer noted that the project will end in September 2019 and there are 3 months remaining.

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

Reviewer 1:
The reviewer said that the project tasks are well aligned with the VTO goals and objectives.

Reviewer 2:
The reviewer agreed that this work greatly supports the DOE's objective to develop high-performance and high-energy-density Li and Li-ion batteries.

Reviewer 3:
The reviewer commented that diagnostic tools provide excellent insights into critical battery materials.

Reviewer 4:
The reviewer found that the project, which is aimed at developing high-energy batteries with lower cost, is highly relevant to overall DOE objectives. The reviewer elaborated that the fundamental degradation mechanism study in this work can provide very important input for future electrode and electrolyte improvement.

Reviewer 5:
The reviewer replied yes, elaborating that the characterization toolset for looking at the degradation of active electrode materials is important for EVs.

Reviewer 6:
The reviewer responded that overall there is good relevance, but added that industry is much moving away from Li-rich, O_2-loss cathode materials because they exhibit a number of performance issues such as voltage fade, low state of charge (SOC), impedance rise, etc. The reviewer added that high-Ni NMCs are much more relevant right now and would encourage the PI to turn these powerful techniques to studying NMC-811 or other high-Ni cathodes.

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

Reviewer 1:
The reviewer praised amazing production from this group for the funding level.

Reviewer 2:
The reviewer commented that given the PI's excellent track record of research progress and the technical challenges in developing these techniques, more resources should be directed toward his work.

Reviewer 3:
The reviewer found that the PI has adequate resources to conduct the proposed research.

Reviewer 4:
The reviewer said the PI has sufficient resources to carry out the proposed work.

Reviewer 5:
The reviewer stated that the resources are sufficient for the proposed tasking.

Reviewer 6:
The reviewer replied resources are sufficient.

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

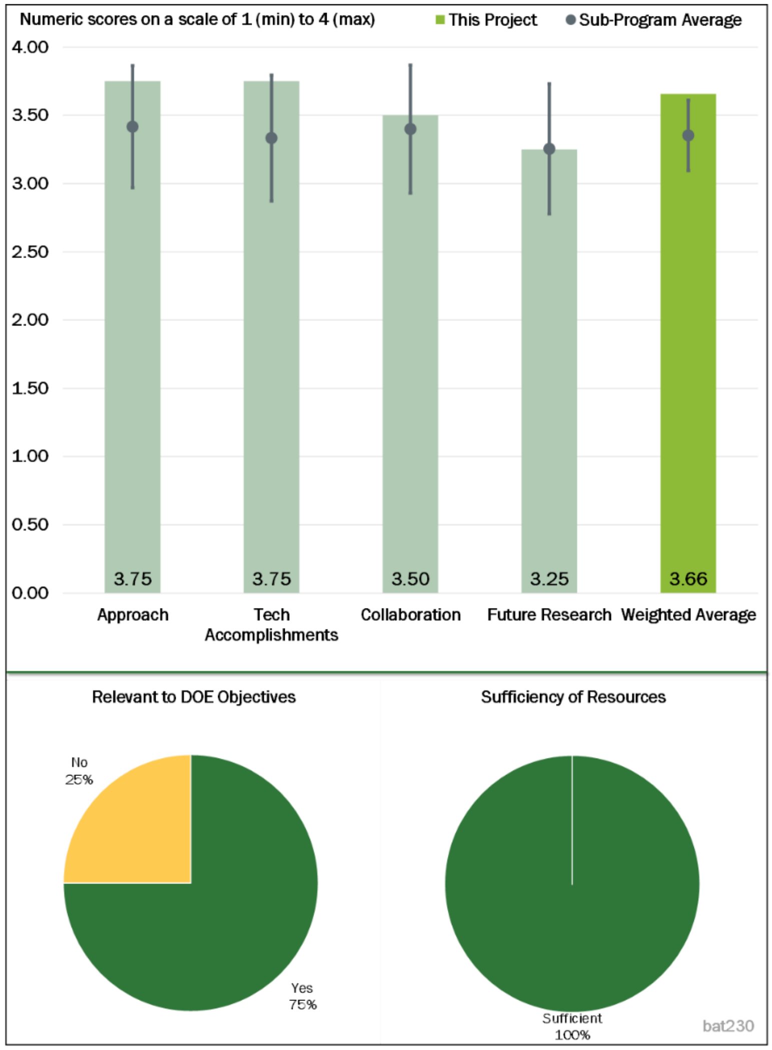

Figure 2-12 – Presentation Number: bat230 Presentation Title: Nanostructured Design of Sulfur Cathode for High-Energy Lithium-Sulfur Batteries Principal Investigator: Yi Cui (Stanford University)

Presenter

Yi Cui, Stanford University

Reviewer Sample Size

A total of 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 the PIs clearly address the key technical barriers such as PS dissolution and the limitation of volumetric capacity of S-based cathode. The reviewer elaborated that the approaches used such as the materials design in nanometer-size length scale, development of high S-loaded PS confinement structure, and PS trapping agent to minimize the PS dissolution are novel and innovative. The PIs also report efficient packing of S in the electrode to maximize the volumetric capacity. The reviewer concluded that in-situ materials characterization techniques in real time to understand fundamental lithiation and delithiation mechanism during the charge and discharge process will provide considerable insight on performance degradation mechanism of the Li-S battery system.

Reviewer 2:

The reviewer said the use of optical microscopy is wonderful.

Reviewer 3:

The reviewer remarked that the research conducted by the PI is always novel and addresses the major challenges confronting battery technology, adding that this project, directed on Li-S, is the same. Several novel techniques to address cell degradation caused by PS and electrode volume expansion were conducted.

Reviewer 4:

The reviewer remarked that the performer identified the relevant issues with Li-S cells and proposed innovative solutions to trap or encapsulate PS.

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 that excellent progress has been made both on the technological and fundamental scientific points of views, which is evidenced from excellent publications in high-impact journals. The reviewer described as clearly an excellent achievement of the PIs that fundamental understanding of PS adsorption and interaction with different types of PS-trapping agents, as well as using oxides and sulfide-based catalyst. The in situ undercooling experiment during electrochemical de-alloying processes of PS to liquid S using non-wetting nucleation site (Ni) is very innovative and novel experiments in solidification science. However, the reviewer added, that in real battery systems, it is expected that the solidification of S will be triggered above room temperature due to the presence of a large number of other heterogeneous nucleation sites such as binder, super P carbon, etc.

Reviewer 2:

The reviewer stated that the performer demonstrated good cycle life with the proposed PS mitigations, albeit with low loadings. The reviewer added that the results of the super-cooled S droplets provided key insights of the S nucleation mechanism that should guide S-cathode design to improve utilization.

Reviewer 3:

The reviewer affirmed that significant progress was achieved this year. Of particular interest and value was the unique investigation where a transparent Li-S cell was fabricated and analyzed using light microscopy. The reviewer added that the study revealed the formation of liquid sulfur on a Ni substrate versus crystalline sulfur on a carbon electrode.

Reviewer 4:

The reviewer described the work as beautiful science but added the relevance to batteries remains to be seen.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that the PIs have developed a strong collaboration with Stanford colleagues, Stanford Linear Accelerator Center (SLAC) National Accelerator Laboratory, and PNNL, which will help to understand fundamental S cycling mechanism and the performance degradation mechanism of Li-S system and help to develop mitigation strategies.

Reviewer 2:

The reviewer remarked there are lots of great collaborators.

Reviewer 3:

The reviewer indicated that the PI is collaborating with various groups including SLAC (Mike Toney) and PNNL (Jun Liu and Jie Xiao).

Reviewer 4:

The reviewer said the performer has demonstrated effective collaboration with SLAC and others from Stanford and PNNL.

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

Reviewer 1:

The reviewer described as well-planned to address the key barriers of the Li-S battery the future work targeting to improve the volumetric capacity and electronic conductivity of the electrode, as well as the development of a high-S loading electrode, and using Si as an anode along with lithium sulfide (Li_2S) as a cathode.

Reviewer 2:

The researcher indicated that the proposed future research is well thought out and demonstrates a clear knowledge of the problems associated with the sulfur cathode.

Reviewer 3:

The reviewer remarked that the project team needs to demonstrate tapping or encapsulation of PS at practical loading of greater than 5 milliamp-hour per square centimeter (mAh/cm^2). The reviewer said the team should also characterize the self-discharge of Li-S cells using their trapped or encapsulated S cathodes.

Reviewer 4:

The reviewer asserted that specific plans for improving volumetric efficiency are lacking.

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

Reviewer 1:

The reviewer commented that developing stable and high volumetric capacity S cathodes is very critical to realizing the DOE target of energy density of 350 Wh/kg for realization of the EV market. The reviewer added that PS confinement and trapping techniques using novel materials design can meet the DOE target goal of energy density and cycle life.

Reviewer 2:

The reviewer found that the project tasks are well aligned with VTO goals and objectives.

Reviewer 3:

The reviewer stated that solving the PS issue and insights on the S nucleation mechanism can provide guidance for a high-performing S cathode.

Reviewer 4:

The reviewer's opinion was that Li-S will not be relevant until a pathway to good volumetric efficiency is at least conceived.

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

Reviewer 1:

With the amount of resources, the reviewer indicated that the performer has developed an extensive and innovative portfolio of trapped or encapsulated S cathodes.

Reviewer 2:

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

Reviewer 3:

The reviewer indicated that resources are sufficient for the proposed tasking.

Reviewer 4:

The reviewer said okay.

Presentation Number: bat247
Presentation Title: High-Energy Lithium Batteries for Electric Vehicles
Principal Investigator: Herman Lopez (Zenlabs Energy, Inc.)

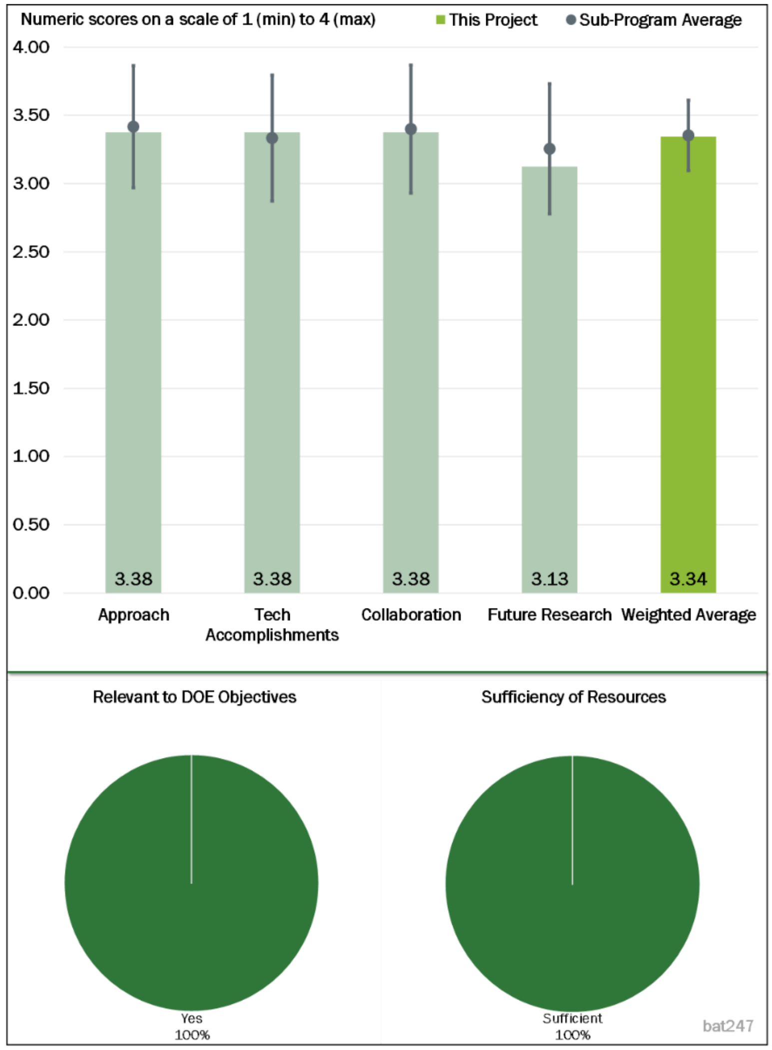

Figure 2-13 – Presentation Number: bat247 Presentation Title: High-Energy Lithium Batteries for Electric Vehicles Principal Investigator: Herman Lopez (Zenlabs Energy, Inc.)

Presenter

Herman Lopez, Zenlabs Energy, Inc.

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 praised the project team's approach and progress as outstanding.

Reviewer 2:

This reviewer commented that the project employed a highly efficient approach, such as optimization of the pre-lithiation process, high-capacity NMC cathode, and SiO_x-C anode materials, as well as selected commercial electrolytes to solve the barriers of cycle-life challenge, large capacity, and reduced battery cost.

Reviewer 3:

The reviewer described the approach as effective and well planned to achieve high-energy Li batteries. The reviewer elaborated that the team has a comprehensive plan to develop high-capacity cathode and anode materials and electrodes, combining the screened commercial electrolytes, separators, and an optimized pre-lithiation process to build high-capacity pouch cells that meet the USABC electric vehicle battery goals for calendar year (CY) 2020.

Reviewer 4:

The reviewer observed that the project approach has identified a materials set that enables higher energy densities through the use of greater than50% SiO_x anodes. The reviewer added that the selection of these materials and the associated manufacturing methods appear to be of good quality based on the low variability of cell performance. Unfortunately, the reviewer added, although scale up to 50 amp-hours (Ah) can be achieved, reduced cost cannot.

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.

Reviewer 2:
The reviewer remarked that excellent progress has been made in the past year. The reviewer elaborated that the team has developed both 11.7 Ah and 50 Ah capacity pouch cells and similar cycling performance is obtained from these cells, adding that all the cells were delivered to the National Laboratory for independent testing. The reviewer added that the team also investigated the OCV and high rate capability of these cells.

Reviewer 3:
The reviewer indicated the progress is pretty good and all the tasks have been completed including the cycle lifetime of 1,000 cycles with 80% capacity retention for 11.7 Ah capacity and 304 Wh/kg.

Reviewer 4:
The reviewer observed that the project has been completed in its fourth year with a 1 year of no-cost extension, adding that cell performance appears good and meets the key metrics of cycle life and rate capability. However, the calendar aging data appear inadequate, as it is conducted over only 12 hours whereas at least 2 months would be desirable. The reviewer also stated that scaling up of cells to 50 Ah has been successful. The reviewer also noted that there are still several performance tests ongoing, despite the project being complete, and therefore it is difficult to assess the true value of the greater than 50% SiO_x anode cell. The reviewer remarked that use of NMC-622 is not particularly competitive, which perhaps is one reason why the 350 Wh/kg target for this project has not been met. The reviewer also remarked that the full materials set in these cells, including electrode formulation and electrolyte composition, should be reported, as well as the conditions of cycle testing (i.e., with pressure plates). Finally, the reviewer stated that the most critical element of this technical program is the cost calculation, which appears very far from the initial estimate due to pre-lithiation and no clear path to improve this.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said that the PI has good collaborations for the electrode development, cell building, and testing.

Reviewer 2:
The reviewer said there is wide project collaboration with several Laboratories, academia, and industrial companies.

Reviewer 3:
The reviewer noted that there are collaborations among Zenlabs and three National Laboratories (Idaho National Laboratory [INL], Sandia National Laboratories [SNL], and NREL).

Reviewer 4:
The reviewer found that the coordination and extent of engagement by each partner across the project team are unclear, adding that most partners are materials manufacturers.

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

Reviewer 1:
The reviewer explained that the team proposes to develop other materials and cells based on these results, and a new program about fast-charge and low-cost Li-ion batteries will be continued. The reviewer added that the proposed work is necessary to move forward.

Reviewer 2:
The reviewer indicated that battery cost may be further reduced after the development of novel electrolytes and a scalable pre-lithiation process.

Reviewer 3:
The reviewer recommended also running some tests in the future work, such as calendar life test and monitoring the cell deformation (thickness change) during cycling, etc.

Reviewer 4:
The reviewer observed that the proposed future work involves mainly completion of cell performance testing. Even though the project has ended, the reviewer said, much of the testing is not complete, and therefore VTO should ensure that this information is reported when available. Furthermore, the reviewer remarked, there are some suggestions for reducing the cost of pre-lithiation, which is a key enabler for this cell, but no clear path forward that would make it viable. The reviewer added that a focus on fast-charge ability (in the new USABC program) could help distinguish this material's set.

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

Reviewer 1:
The reviewer affirmed that the project is highly relevant and supports DOE objectives, because it aims to develop high-energy batteries that meet the USABC electric vehicle battery goals.

Reviewer 2:
The reviewer said that this research is on high-performance Li-ion batteries with high-capacity electrodes (NMC and SiO_2-C), adding that it is a promising choice for an electric vehicle battery.

Reviewer 3:
The reviewer stated that this project aims to develop high-energy density, low cost, and long cycle life Li-ion batteries, which are consistent with DOE's guidance.

Reviewer 4:
The reviewer remarked that while this project addresses the need to further develop Si-containing anodes for high-energy density cells, it does not solve the key issue of cost.

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

Reviewer 1:
The reviewer replied that the resources are sufficient for the successful completion of this project.

Reviewer 2:
The reviewer found that all program milestones and gates have been completed, as scheduled, and final cells have been delivered.

Reviewer 3:

The reviewer agreed that the resources for the project are sufficient to achieve the target.

Reviewer 4:

According to the reviewer, the resources for this project are sufficient. More time will likely be needed for completion of testing.

Presentation Number: bat252
Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Project Completion Highlights, Part I
Principal Investigator: Jason Croy (Argonne National Laboratory)

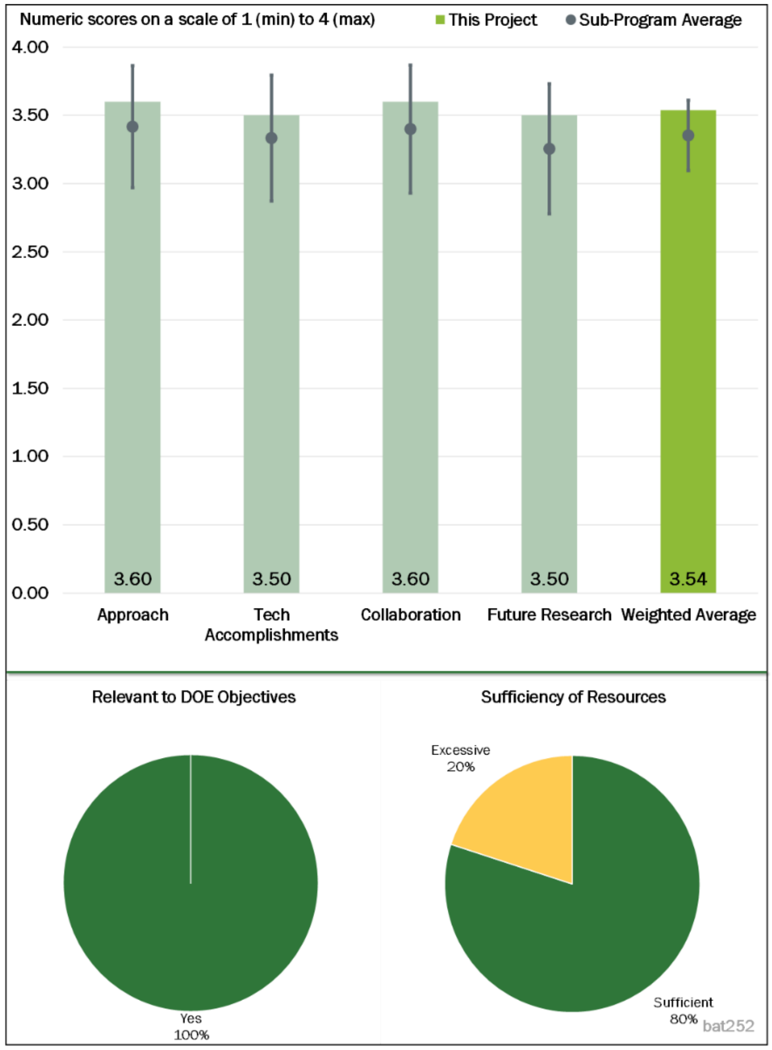

Figure 2-14 – Presentation Number: bat252 Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Project Completion Highlights, Part I Principal Investigator: Jason Croy (Argonne National Laboratory)

Presenter
Jason Croy, 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 observed that the project looked at issues related to various NMC cathode materials systems such as segregation issues, bulk structural changes, and stabilization using electrolyte additives. The reviewer concluded that the approaches—which involved the use of experiments combined with theory—are all excellent.

Reviewer 2:
The reviewer offered that the technical approach taken by the project was focused and in depth to make progress in studying barriers including capacity drop related to anodes and impedance increase related to cathodes that affect high-energy and high-voltage Li-ion battery life.

Reviewer 3:
Good approach, the reviewer said, and well designed.

Reviewer 4:
The reviewer presented three observations: First, the standardization of materials and test protocols is critical, and the reviewer was glad to see that being addressed, adding we need to proliferate that in the industry. Second, the model systems, especially the varying compositions and particles with different facets, are a great idea. The reviewer hoped the project team is able to study this material set including with different coatings, electrolytes, etc. However, the reviewer thought this needs to be more strongly linked to industrially relevant materials, adding that this is easy to say, hard to do. Third, there is an excellent approach to crosswalk evaluation with LFP and doping in Mn with ligands to the electrolyte.

Reviewer 5:
The reviewer stated that that the approach is effective with a significant effort dedicated to the standardization and protocol development. The reviewer added that it would have helped to establish baselines based on the current industry acceptable charging voltages and select "High Voltages" based on industry targets and safety expectations. The reviewer remarked it is understood that the complexity of the task and changing industry trends make it very difficult to select and focus on the specific chemistry; thus, results presented were open ended.

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 as outstanding the work toward identifying major challenges and developing modeling and experimental programs to address. Most importantly, is searching and testing new materials and new hypotheses that could find practical use in industry, for example, electrolyte additives work.

Reviewer 2:
The reviewer commented that the project yielded systematic understanding of NMC cathodes and their behavior. The reviewer elaborated that experimental results combined with theoretical studies yielded fundamental insight into Ni and cobalt (Co) segregation based on different facets, interaction with coatings such as alumina, and the effect of electrolyte additives.

Reviewer 3:
The reviewer found that standardization of coin and pouch cells was well executed with good use of DFT calculations. The reviewer added that the research could use some more patent submissions.

Reviewer 4:
The reviewer found that significant progress has been made in this project and especially progress on some promising strategies on how to stabilize NMCs at high voltages, but added that it was unclear if the project can provide some potential direction (at least theoretically) on how to stabilize even lower cobalt NMCs that DOE is interested in.

Reviewer 5:
Given the resources devoted to this program over the last four years, the reviewer would have liked to see more substantial performance outcomes. The reviewer thought there was good progress on standardization and model systems, but was unsure if technology can help materials or battery manufacturers make better products. The reviewer asked, what should be done differently to make high Ni, high voltage materials work better. The answer, the reviewer stressed cannot only be to find a new electrolyte additive. Noting that it seems coating is one solution, the reviewer mainly heard that aluminum oxide (Al_2O_3) does not work. The reviewer inquired about what works and why.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found excellent collaboration among experimentalists, theorists, and several partners.

Reviewer 2:
The reviewer gave overall kudos to DOE, elaborating that the interaction among teams and members of the teams is truly genuine with a clear understanding of the goals and a desire to contribute and help each other. The reviewer added that the publication lists are impressive.

Reviewer 3:
The reviewer found good collaboration among the National Laboratories.

Reviewer 4:

The reviewer explained that the team consisted of four Laboratories with over 45 people working on the project in one form or another. The reviewer hoped the standardization of materials and test protocols was used by all. The reviewer asked if the online database of results is accessible to the public. The reviewer would have liked to see more industry participation in this effort, adding that could have brought a lot of insight into what approaches are commercially relevant.

Reviewer 5:

The reviewer stated that close collaboration within team members is obvious, but it was unclear how each team member is contributing to the 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 found that the proposed future research is adequate and good. The reviewer hoped to see industry partners included in a team for the future work to facilitate technology transfer into a potential product.

Reviewer 2:

The reviewer noted that the project has ended.

Reviewer 3:

The reviewer said the project has ended.

Reviewer 4:

The reviewer commented that future work is the subject of another project as this has been completed.

Reviewer 5:

The reviewer stated that this project is complete. The reviewer added that what would be very appreciated by industry is the final report outlining the findings and how what was learned could be applied to Li battery chemistries of the future.

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

Reviewer 1:

The reviewer agreed that the project supports the DOE objectives very well to further increase Li-ion battery energy density by studying barriers on high-energy and high-voltage Li-ion cells.

Reviewer 2:

This reviewer affirmed that the project supports the overall DOE objective by investigating several aspects of batteries, adding that it integrated both theoretical work and experimental work through collaborations.

Reviewer 3:

The reviewer commented that any knowledge, fundamentals, and improvements identified for these high-energy battery materials can ultimately help DOE achieve energy storage targets for automotive applications.

Reviewer 4:

The reviewer said this project is about understanding NMC cathode materials and their stability with cycling and at various depths of discharge and voltages.

Reviewer 5:
The reviewer remarked that it is important to compare the best-case scenario to the existing situation, explaining this would stimulate funding of the projects that would help to close the gap and achieve cost targets of dollars per kilowatt-hour.

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 a very good match of the skill set among the team leading to a good alignment.

Reviewer 2:
The reviewer commented that the resources were adequate.

Reviewer 3:
The reviewer stated that this project has been finished.

Reviewer 4:
The reviewer replied that the resources seemed sufficient but added there may be a need for high-temperature thermal testing.

Reviewer 5:
The reviewer remarked that given the amount of resources (people and technology) and time (4 years) on this effort, there should have been more commercial impact. The reviewer asked how the knowledge gained can advance United States (U.S.) industries in the manufacture of materials and cells.

Presentation Number: bat253
Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Project Completion Highlights, Part II
Principal Investigator: Dan Abraham (Argonne National Laboratory)

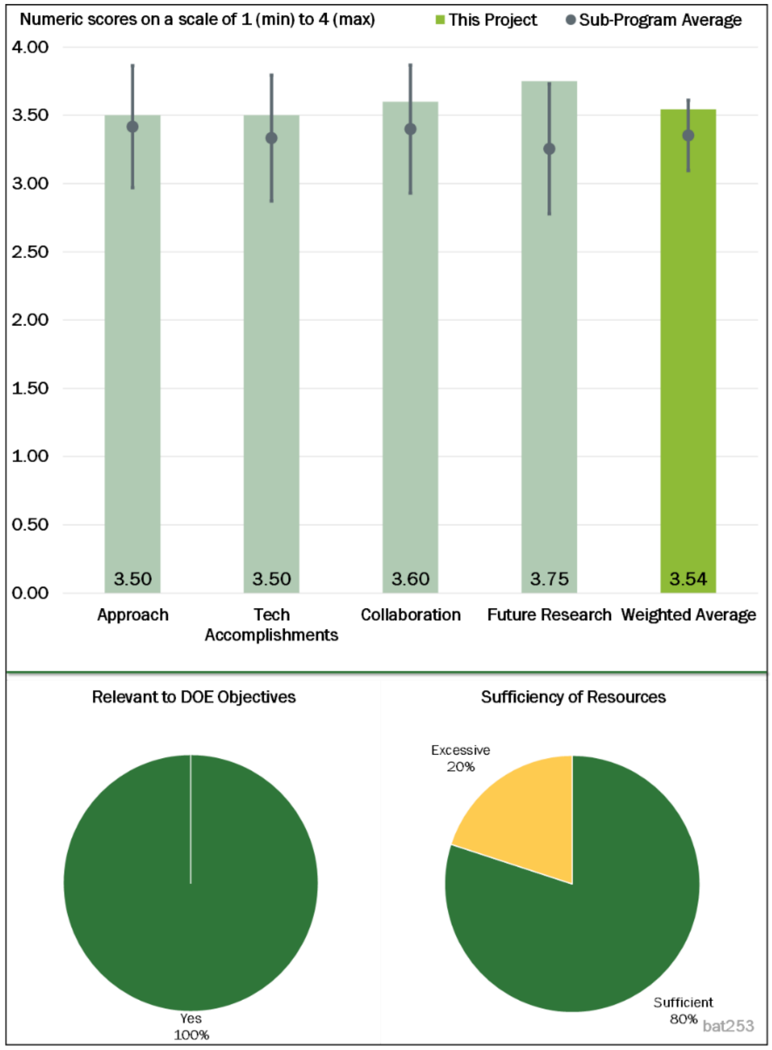

Figure 2-15 – Presentation Number: bat253 Presentation Title: Enabling High-Energy, High-Voltage Lithium-Ion Cells for Transportation Applications: Project Completion Highlights, Part II Principal Investigator: Dan Abraham (Argonne National Laboratory)

Presenter

Dan Abraham, 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 said the project addressed the technical barriers well with several different approaches to determine factors that contribute to capacity fade and impedance rise.

Reviewer 2:

The reviewer remarked that this is part 2 of BAT252 so the comments are very similar and said the approach is effective; there has been significant effort dedicated to standardization and protocol development. The reviewer said it would have helped to establish baselines based on the current industry-acceptable charging voltages and select “High Voltages” based on industry targets and safety expectations. There was excellent research discipline demonstrated and answers to some of the research questions were provided.

Reviewer 3:

The reviewer commented the approach was good with good integration of theoretical and experimental work. The reviewer added it might need a little more theoretical research, like the development of Figure of Merit (FOM).

Reviewer 4:

The reviewer observed that this work is also a systematic study of high-voltage cathode materials and their behavior with cycling at different potentials, electrolyte additives, and aging conditions. The data are fairly interesting. The reviewer stated that the results with additives are useful for developing next-generation electrolytes. This project seems to set a stage for a continued project on electrolytes for high-voltage cathode materials.

Reviewer 5:
The reviewer said the approach to improving high-energy materials was good, but asked what is new here. The speaker kept referring to approaches that had been discussed for many years prior. The reviewer thought the cathode and anode recipes are outdated. No one uses 90% active material in the cathode. The reviewer was concerned that the results obtained on these systems may not have broader relevance.

The reviewer liked the FOM approach to finding electrolyte combinations. There needs to be more efforts like this to prevent electrolyte research from being completely trial and error. The reviewer suggested a message that electrolyte additives may form products within the formulation, which may be beneficial or detrimental, and that needs to be proliferated. Industry knows this, but many others do not.

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 the project as outstanding work toward identifying major challenges and proposing solutions. Most importantly, the project team searched and tested new materials and new hypotheses that could find practical use in industry, for example electrolyte and additives work.

Reviewer 2:
The reviewer found lots of good technical progress has been made in this project. Cathode impedance rise is considered one of the major factors for high-energy and high-voltage Li-ion cell life. It was unclear to the reviewer if cathode impedance rise or Li-trapping in the negative electrode is the major factor to limit cell life.

Reviewer 3:
The reviewer commented that the project yielded some interesting observations about increasing impedance, loss of capacity, and the use of additives and their role in decreasing gas evolution and improving durability. Some of the results with electrolyte additives are definitely useful. Also, the reviewer said the protocol on calendar life (with aging) seems interesting but needs a little bit more rationale on why that protocol makes sense. According to the reviewer, it is also important to understand what that protocol means for long-term performance of the battery.

Reviewer 4:
The reviewer mentioned that technical accomplishments seemed good, adding that the TM dissolution research was interesting. The reviewer said it would be interesting to have seen theoretical DFT predictions to confirm findings.

Reviewer 5:
The reviewer would have expected more impact in a 4-year project with over 40 contributors and all the resources of the U.S. National Laboratories to bring to bear. The reviewer said the large number of publications is good and so communication of knowledge was good. But it still involved a relatively small number of electrolytes (42 different electrolyte systems) over the time frame. The reviewer asked which one industry should use for which cathode. The reviewer thought a lot of good tools and methodologies were set up for the "next" project but would have liked more results from this one.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said the coordination among the group is excellent.

Reviewer 2:
The reviewer replied that collaboration within the team looks strong and effective.

Reviewer 3:
The reviewer remarked that the interaction among the teams and members of the teams is truly genuine with a clear understanding of the goals and desire to contribute and help each other. The reviewer described the publication lists are impressive.

Reviewer 4:
The reviewer found good collaboration with DOE National Laboratories but suggested it might be worthwhile to team with an industry partner in the future.

Reviewer 5:
Noting that it is challenging keeping a large team at multiple sites on track, the reviewer said it seems this was done well. Again, the standardization is critical to being successful here. The reviewer would have liked to see input and participation by industry, especially when one of the outcomes is that electrolyte time studies are very important in the identification of beneficial species in the formulation.

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:
Though this project is complete, the reviewer said the team made an effort to select and summarize concepts and ideas applicable for the new Cathode Program. Some of the results clearly show that development of the Mn- and Co-free cathodes is possible. It was a great job.

Reviewer 2:
The reviewer stated the proposed future research is reasonable and hoped to see the ideas developed in this project such as FOM can be applied to next-generation cathode study such as low-Co cathode.

Reviewer 3:
The reviewer stated that the project has ended.

Reviewer 4:
The reviewer replied the project ended.

Reviewer 5:
The reviewer said the project is already finished.

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

Reviewer 1:
The reviewer agreed the project supports the overall DOE objective of advancing battery technology.

Reviewer 2:
The reviewer said the project supports the DOE objectives by studying the power and energy loss of high-energy and high-voltage Li-ion cells.

Reviewer 3:
The reviewer commented that we need more fundamental knowledge and advancement of technologies to make high-energy battery materials work and that this project contributed to the knowledge base.

Reviewer 4:
The reviewer said this is certainly an important project and should be of strong interest to industry.

Reviewer 5:
The reviewer explained the project has focused on examining and addressing the energy and power loss of the lithium bis(oxalato)borate (LiBOB) and provided some hypothesis and mechanisms that would help to design the remedies.

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 a very good match of the skill set leading to a good alignment.

Reviewer 2:
The reviewer stated resources were good.

Reviewer 3:
The reviewer concluded that resources were adequate.

Reviewer 4:
The reviewer said this project has been finished

Reviewer 5:
The reviewer’s comment relates back to the outcome, which—although there were lots of good publications and some patent applications—were a bit lacking in terms of real improvements that can be applied commercially. This was really a great team with world-class resources.

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

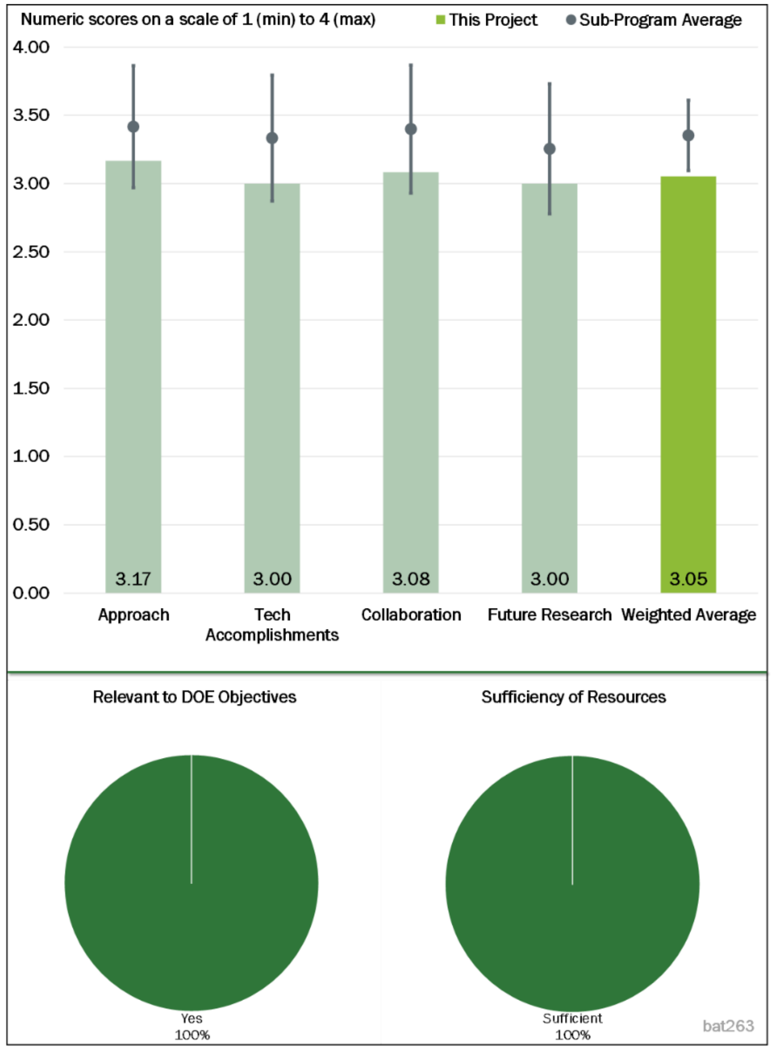

Figure 2-16 – Presentation Number: bat263 Presentation Title: PPG: Electrodeposition for Low-Cost, Water-Based Electrode Manufacturing Principal Investigator: Stuart Hellring (PPG)

Presenter
Stuart Hellring, PPG

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 described the approach as a solid alternative approach to traditional PVDF slot die coating. The reviewer added that a project like this needs more support on modeling to show the economics of it. The reviewer elaborated that it is also a difficult project for people to realize value in, as to most researchers, coating battery electrodes appears to be a trivial process, but for manufacturers it is often one of the most expensive steps.

Reviewer 2:
The reviewer suggested the water-based processing could reduce the cost for cathode manufacturing. The reviewer remarked that the biggest challenge for water-based cathode processing is the reaction between the cathode materials and water. Though the reactions may be not faster or significant, the products from the reaction may have significant impact on electrode performance. As shown in Slide 8, the rate capability of an electrode coated by the water process is not good: The capacity at 1 C is only about 60% of that at 0.1 C. The adhesion should also be compared with NMP-based processing.

Reviewer 3:
The reviewer described the approach as strongly innovative, but with considerable risk. The reviewer added that feasibility, from a timing perspective, was probably not best understood at the onset of the program.

Reviewer 4:
If successful, the reviewer remarked, the electrodeposition approach would significantly reduce waste and cost associated with production of Li-ion battery electrodes.

Reviewer 5:
The reviewer said the project is well-designed and the approach feasible; however, it still remains to be seen if the approach will be successful.

Reviewer 6:
The reviewer stated that electrodeposition is an interesting technique to explore as an electrode-coating system. The reviewer added that there are many concerns that would need to be addressed as the electrode formulation is a multicomponent system, which would make this more challenging than typical electro-coating applications.

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 that the investigation team has made great progress and has uncovered some of the significant challenges to this approach. They have tackled the challenges appropriately, and evidence indicates they will continue to do so.

Reviewer 2:
The reviewer noted that fundamental work has been completed to accomplish successful LFP coatings. Key next steps in scale-up and steady-state operations need to be reviewed. The reviewer explained that lack of consistency in bath formulation and dry coating need to be solved along with the impact of the slurry prep on cell performance.

Reviewer 3:
The reviewer said it was a good demonstration of process potential, adding that the reality is that a major cost improvement would be a necessary requirement to consider longer term development. This should be part of the overall plan in the go/no-go tree.

Reviewer 4:
The reviewer affirmed that good progress was made on a bench scale but added that some challenges remain for the pilot-scale operation, especially with high-Ni cathodes.

Reviewer 5:
While the water-based coating results have been promising, the reviewer remarked that the performance with the pilot coater is well below the baseline material. Additionally, the reviewer posed two questions that arose but that were not addressed: First, the reviewer asked how the water-based electrochemical electrode compares to other aqueous-prepared electrodes (CMC, polyacrylic acid [PAA], alginate, and water-based PVDF). Second, the reviewer wanted to know what the rate of deposition is, compared to the traditional slurry preparation process.

Reviewer 6:
The reviewer stated that there is not enough discussion, comparison, or data to justify how the processing reduces the cost and avoids toxic material exposure.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer replied that partners appear well coordinated with all delivering their required products.

Reviewer 2:
The reviewer stated that the PPG team has extensive experience in coordinating projects like this one. They are also collaborating with industrial partners and DOE Laboratories.

Reviewer 3:
The reviewer was glad to see prestigious partners involved: Navitas Systems, ORNL, and Argonne National Laboratory (ANL).

Reviewer 4:
The reviewer replied that collaboration and coordination seem to be reasonable.

Reviewer 5:
The reviewer stated that collaboration is acceptable.

Reviewer 6:
The reviewer remarked that collaboration was not evident in this project, but the team appeared to utilize collaborators and partners to fulfill areas they were not subject matters experts in. The reviewer had no issue with the amount of collaboration but just that there was not a lot of it.

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

Reviewer 1:
The reviewer indicated the project is almost complete and the team is working on finishing up loose ends.

Reviewer 2:
The reviewer stated that an effort is needed to evaluate electrode quality comparing it to NMP-based processing such as adhesion, stability, uniformity, etc.

Reviewer 3:
The reviewer suggested a little more emphasis on the future deliverables' targets would help and to be more metric oriented.

Reviewer 4:
The reviewer reiterated that substantial cost-reduction potential should be projected to advance technical development.

Reviewer 5:
The reviewer indicated that the future focus is on pilot coater redesign, which makes sense. The reviewer suggested the project team should also try to learn more about fundamental limitations of a water-based approach.

Reviewer 6:
The reviewer commented that the success of the project depends on the "pilot coater redesign" and "improved downstream curing." The reviewer added that no details of exactly how these might be approached were given, so it is impossible to evaluate the likelihood of success. The coater redesign is particularly vague, raising doubts that the issue will be effectively overcome.

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

Reviewer 1:
The reviewer said that finding new ways to produce electrodes with less waste and at lower cost is critical to achieving DOE goals.

Reviewer 2:
The reviewer found the project to be highly relevant to securing a domestic energy storage supply, elaborating that this technology, if translated and maintained in the United States, could provide domestic manufacturers with a lower cost method that would allow them to be cost competitive with overseas manufacturers due to the reduction in labor. While it lacks the flash of National Laboratory projects with their synchrotrons, the reviewer concluded that this project aligns far better with providing meaningful benefit to the United States.

Reviewer 3:
The reviewer agreed that this project supports the overall DOE objectives to reduce manufacturing cost for Li-battery processing and reducing environmental impact.

Reviewer 4:
The reviewer said the approach has the possibility to simplify cathode electrode fabrication, with lower overall costs and net carbon emissions.

Reviewer 5:
The reviewer pointed out that electrode-coating technology is a major cost driver in Li-ion battery production and that this is a legitimate technique to explore to the point where potential cost improvement can be demonstrated.

Reviewer 6:
The reviewer wrote that improved battery manufacturing could well decrease costs of EVs.

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

Reviewer 1:
The reviewer had no comment to the question but was impressed with the breadth of research completed for the project cost.

Reviewer 2:
The reviewer said that resources and the partnership are sufficient to perform the proposed work.

Reviewer 3:
The reviewer replied the resources are sufficient.

Reviewer 4:
The reviewer had no major concerns with resources.

Reviewer 5:
The reviewer stated that there is no indication that there has been a shortage of resources.

Reviewer 6:
The reviewer responded that this is a difficult question to answer in the absence of more detailed descriptions of what the future work will entail.

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

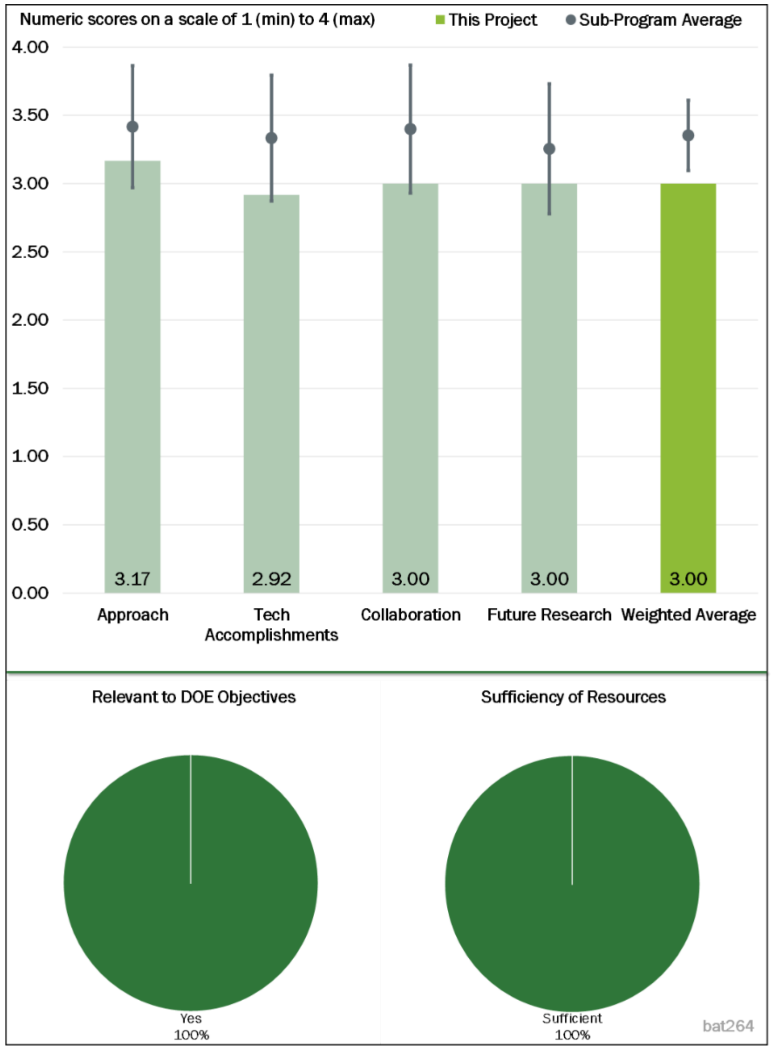

Figure 2-17 – Presentation Number: bat264 Presentation Title: High-Performance Lithium-Ion Battery Anodes from Electrospun Nanoparticle/Conducting Polymer Nanofibers Principal Investigator: Peter Pintauro (Vanderbilt University)

Presenter

Peter Pintauro, Vanderbilt 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 said the approach is very innovative and that it has been shown to be effective.

Reviewer 2:

The reviewer said that using electrospun fibers to improve the anode performance is a very innovative approach that can address some of the key barriers to anode performance.

Reviewer 3:

The reviewer stated it was a novel approach to silicon processing, which may provide benefits.

Reviewer 4:

While the technique of electrospinning is an interesting option associated with Si-anode production, the reviewer remarked that there are many questions that need addressing. Issues of fundamental performance of electrospun Si, impact of solvent on surface state, uniformity of porosity, etc., are all questions that could benefit from more attention. Finally, the reviewer said, as with all technique developments, a level of cost projection is necessary to determine whether any commercial relevance exists.

Reviewer 5:

The reviewer stated that the approach may stabilize the structure of the silicon electrode but could not improve cycling efficiency, so it is less likely to address the capacity-fading issue.

Reviewer 6:

While finding the approach to be reasonable, however, the reviewer said it offers little hope for the issue of long-term less-than-optimal CE of Si electrodes, an issue that must be addressed to have any practical impact.

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 the project team was able to demonstrate high-capacity anodes when using electrospun fibers, especially when carbon was added.

Reviewer 2:
The reviewer said the progress was good. One item missing, according to the reviewer, is related to how this approach can be converted to a practical anode design suitable for a full-size cell.

Reviewer 3:
The reviewer offered the following observations: The barriers to address were to improve capacity fade and a goal was 200 cycles at 0.1 C, which would demonstrate effective compensation for Si expansion: however, the majority of the testing was performed at 1 C with much lower Si utilization and thus less expansion per particle. The reviewer said more long-term full lithiation testing should be performed, such as a constant current/constant voltage (CC/CV) charging profile to ensure full lithiation.

One of the biggest problems with Si nanoparticles is poor long-term CEs compared to graphite. The reviewer asked how the electrospun fibers compare in CE to traditional Si electrode preparation.

The reviewer said there is no mention of volumetric capacity for the cells, and asked what an estimated volumetric capacity for a pressed Si-PAA electrospun fiber electrode is. If the porosity is too high, as it appears to be, the volumetric capacity, equally (or more so) important as gravimetric capacity, will not be impressive.

Reviewer 4:
The reviewer stated that the authors have formed mats of electrospun Si and carbon. While this is interesting, the project team has not successfully built it into an electrode that can compete with a graphite electrode in areal capacity terms and has any meaningful cycle life. This does not address their barriers addressed on their slide of capacity fade and high volumetric energy density.

Reviewer 5:
The reviewer remarked that there is a lot of PAA or other binders used in the process to help stabilize the structure, but that these contribute little to capacity and CE. The cycling life is still very poor compared to other Si electrodes reported in literature or by industry.

Reviewer 6:
The reviewer commented that while process technology provides interesting options, the ability to evaluate from a fundamental electrode-performance perspective is not terribly high and is mostly empirical. The reviewer added that issues of post-treatment by compression and solvent exposure are lightly dealt with and likely more complicated than portrayed.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the team collaboration is excellent and it includes university, National Laboratory, and industrial partners.

Reviewer 2:
The reviewer found relevant prestigious partner involved.

Reviewer 3:
The reviewer said that the small collaboration base appears acceptably managed. Actual electrode characterization could benefit from identification of a collaboration partner.

Reviewer 4:
The reviewer observed some work with National Laboratories and added that the authors could have used more expertise in battery systems to try and better understand cycle life and how this method does not improve it.

Reviewer 5:
The reviewer found limited collaboration but it could well be sufficient given the nature of the project.

Reviewer 6:
The reviewer said that collaboration with ORNL was not as clear as it should be.

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 one of the remaining issues is how to reduce amount of binder used in electrodes and recommended that the team should look for practical ways to achieve that goal.

Reviewer 2:
The program is nearing completion, the reviewer remarked, and future work was not clear. If the investigator can provide a convincing description on how a practical anode can be made, then this project would merit continued work.

Reviewer 3:
The reviewer said the project is near completion, but no future work is given.

Reviewer 4:
The reviewer replied that future research is not addressed.

Reviewer 5:
The reviewer said there is no proposed future research.

Reviewer 6:
The reviewer replied it is not applicable (N/A), as the project ends soon.

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

Reviewer 1:
The reviewer stated that improving anode capacity is critical to achieving DOE goals.

Reviewer 2:
The reviewer commented that Si is a very promising candidate anode material to boost energy density by 10%-15% for Li-ion batteries.

Reviewer 3:
The reviewer indicated that Si-based anode systems are likely an important pathway in Li-ion energy-density improvement.

Reviewer 4:
The reviewer remarked that the 600 milliamp-hours per gram (mAh/g) is a little low, but it can be considered very successful if the cell-level design and cost targets can be demonstrated by analysis. The reviewer asked the team to please show the performance values (Wh/kg and Wh/L) for a 50-Ah cell (possibly using BatPac model) as well as an estimate for cost savings over a conventional electrode.

Reviewer 5:
The reviewer said Si anodes could contribute to higher capacity batteries and thus better EV performance.

Reviewer 6:
The reviewer replied that there is novel processing, but the economics are not well understood, and added that the success of the project is to be determined as life and energy did not improve, but the study of the processing may spark future work.

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 goals are within the capability of the budget, adding that the budget is quite modest, and any extension of this work would require more funding.

Reviewer 2:
The reviewer replied the resources are sufficient.

Reviewer 3:
The reviewer observed no issues.

Reviewer 4:
The reviewer said the project is ending in September 2019.

Reviewer 5:
The reviewer replied the project could have benefited from a larger scope on electrochemical testing but likely out of budget.

Reviewer 6:
The reviewer stated the resources are sufficient to perform the approach to stabilize Si-anode structure, but more should be focused on CE improvement. In the reported results, the reviewer remarked that the dramatic capacity loss at the beginning prevents practical application.

Presentation Number: bat265
Presentation Title: Development of Ultraviolet Curable Binder Technology to Reduce Manufacturing Cost and Improve Performance of Lithium-Ion Battery Electrodes
Principal Investigator: John Arnold (Miltec)

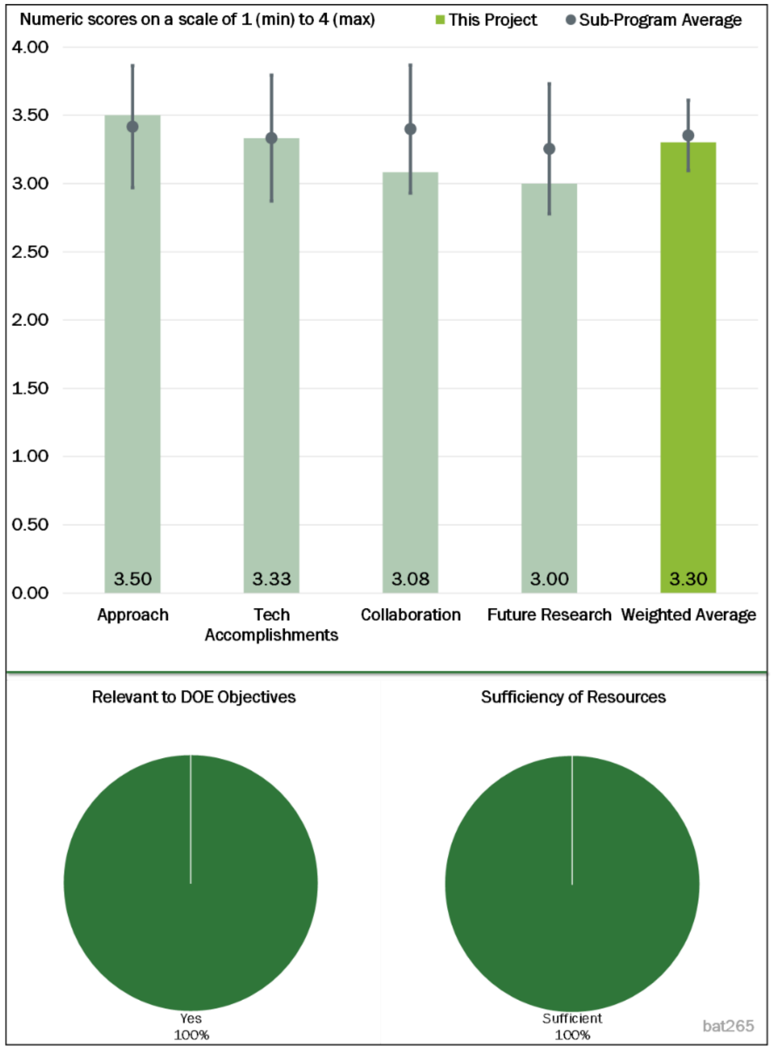

Figure 2-18 – Presentation Number: bat265 Presentation Title: Development of Ultraviolet Curable Binder Technology to Reduce Manufacturing Cost and Improve Performance of Lithium-Ion Battery Electrodes Principal Investigator: John Arnold (Miltec)

Presenter
John Arnold, Miltec

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 described the potential of UV binders as incredible and added that this is a project that could significantly reduce conversion and capital cost of battery manufacturing. The reviewer stressed that DOE needs to focus on supporting more projects of this type and less fundamental science.

Reviewer 2:
The reviewer said the solvent-free process and UV-cure method might be able to reduce the cost for electrode processing and make it possible to coat an electrolyte at a much faster speed.

Reviewer 3:
The reviewer described the approach as a great effort in implementing an innovative manufacturing process and added that the principal investigator also understood how the process could be improved with future work.

Reviewer 4:
The reviewer remarked that developing a fast, safe, and cheap way to make electrodes is important for advancement of battery technology. The UV-curable approach is a unique approach.

Reviewer 5:
The reviewer said the approach is reasonable, well thought out, and potentially feasible.

Reviewer 6:
The reviewer described it as a legitimate approach to an alternative curing process through the elimination of NMP and traditional drying. More attention to physical parameters and performance as compared to a traditional control would be useful.

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 electrodes were coated successfully at different speeds and evaluated in coin cells and pouch cells for comparison.

Reviewer 2:
The reviewer said the focus on projecting cost improvement is admirable. The reviewer elaborated that the curing-process development appears well in hand and the demonstration of multi-layer structures is quite interesting. More comparison to conventional control will be necessary to a develop better understanding of the pros and cons.

Reviewer 3:
The reviewer found some missing data specific to cyclability and calendar life, but otherwise it is very encouraging.

Reviewer 4:
The reviewer said the project team was able to demonstrate layered electrodes, which is a promising approach. Some challenges remain with achieving the desired electrode composition with less carbon and binder.

Reviewer 5:
The reviewer noted that validation in pouch cells has been completed and it shows reasonable energy, but the cycle life is poor. The results would benefit from a baseline cell to determine if the life is impacted by the novel research or if this is simply a cell chemistry with poor life. The reviewer added that the dual-layer coating with power and energy layers is novel and does show some benefits but again the baseline is not well understood.

Reviewer 6:
The reviewer remarked that the claimed cost savings are impressive but impossible to verify due to a lack of details. The cell performance is generally good, but capacity fade is too large and needs significant improvement. The first-cycle CE appears to be missing from the graphs (Slide 7), off the bottom of the graph, giving some reason for skepticism.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the team included industrial and National Laboratory partners.

Reviewer 2:
The reviewer agreed that coordination was clear with a well-functioning team. However, the specific contributions of each partner could have been made clearer within the presentation material.

Reviewer 3:
The reviewer suggested that collaboration with a commercial battery manufacturer, if possible, might be beneficial.

Reviewer 4:
The reviewer said this is not a collaborative project, but the PI did utilize National Laboratories for assistance in cell building.

Reviewer 5:
The reviewer noted the team worked with a partner, but it could be better if working closer with a partner in the Li-ion battery industry for better evaluation of cell performance, compatibility with state-of-the-art electrode materials, and electrolytes.

Reviewer 6:
The reviewer found collaboration acceptable at this level, as with other programs in this section, adding that this is a somewhat empirical approach of build-and-test. The reviewer suggested that a collaboration that included more fundamental electrode characterization would be 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 found that while excellent progress was made, the areas of continued improvement are also clear. The reviewer encouraged the principal investigator to continue the electrical characterization of the current electrodes and then evaluate higher energy materials.

Reviewer 2:
The reviewer replied that moving toward more collaboration with OEM partners is a wise, stated goal.

Reviewer 3:
The reviewer noted the project has ended.

Reviewer 4:
The reviewer commented N/A as the project is ending.

Reviewer 5:
The reviewer suggested future work should address the remaining challenges related to electrode uniformity and porosity control.

Reviewer 6:
The reviewer replied that future work is listed but vague. It is clear this work requires interest from a cell manufacturer to gain traction, but the state of the data is not complete to necessarily gain that endorsement. The reviewer suggested the PI should focus on nearer term future work, which shows their process against a clear and strong baseline.

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

Reviewer 1:
The reviewer stated that developing a faster and cheaper way to produce electrodes is critical to achieving DOE goals.

Reviewer 2:
Yes, the reviewer said, adding that it is very important to reduce the processing cost to make the Li-ion battery processing in the United States environmentally friendly and cost effective.

Reviewer 3:
The reviewer indicated the principal investigator demonstrated the cost reductions and the target performance.

Reviewer 4:
The reviewer found it to be another legitimate technique that could simplify electrode production with the possibility of more custom tailoring of the structure.

Reviewer 5:
The reviewer replied that cheaper battery manufacturing could lower cost of EVs and promote adoption.

Reviewer 6:
The reviewer commented that this project can support a competitive advantage to U.S. cell manufacturers if the technology is picked up, adding that DOE should focus on more near-term impact projects such as this and less fundamental 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 said the demonstration appeared to be quite advanced and indications are the resources were used efficiently.

Reviewer 2:
The reviewer found collaboration and capacity of Miltac as sufficient to complete the milestones.

Reviewer 3:
The reviewer said the resources are sufficient.

Reviewer 4:
The reviewer noted the project has ended on January 3, 2019.

Reviewer 5:
The reviewer had no issues, but suggested that the investment for the next steps could be considerable.

Reviewer 6:
The reviewer replied that no information on resource utilization was given. The reviewer added that a National Laboratory supported cell builds.

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

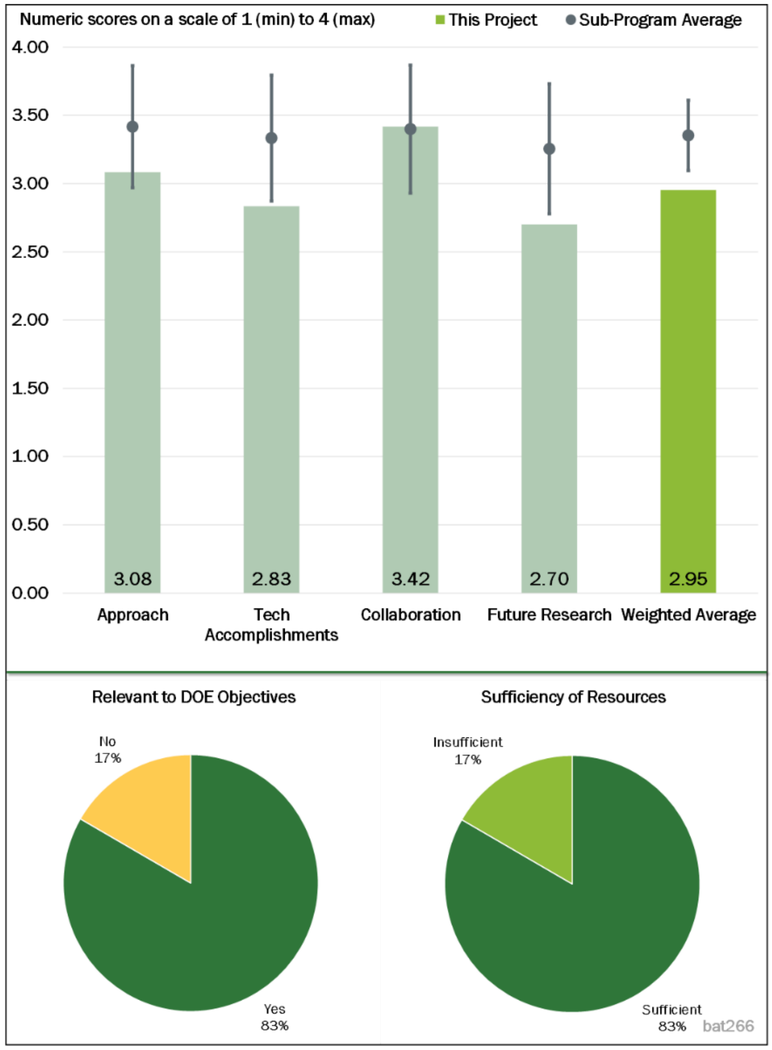

Figure 2-19 – Presentation Number: bat266 Presentation Title: Co-Extrusion (CoEx) for Cost Reduction of Advanced High-Energy-and-Power Battery Electrode Manufacturing Principal Investigator: Ranjeet Rao (PARC)

Presenter

Ranjeet Rao, PARC

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 observed that this project hits an area that is not commonly looked at and added that structuring the electrode could provide clear advantages. This reviewer noted that the PI has leveraged expertise in coating project, which is an excellent approach.

Reviewer 2:

The reviewer found the project to be well designed and the approach is reasonable.

Reviewer 3:

The reviewer suggested that co-extrusion could be a promising approach to produce electrodes with higher energy density.

Reviewer 4:

For the barriers targeted, the reviewer found that the approach demonstrated achievement of those goals. The reviewer added that more cell information would always be preferred, particular in hybrid pulse power characterization (HPPC) and cyclability data.

Reviewer 5:

The reviewer noted that co-extrusion is a legitimate technique to explore in terms of cathode production. The program in question is at an early stage of development. While the goal of producing thick electrode structures is admirable, the reviewer said there are perhaps a few steps missing in the development. It seemed to the reviewer that a stage of development that produced co-extrusion (Co-Ex) structures on par with the baseline structures (loading and thickness) could have provided some direct indication whether there was any technical benefit to the Co-Ex process versus the standard process. Further down the line, while the introduction of electrolyte channels is an interesting feature capability of the process, it could be helpful to produce with and without channels to understand just how important they are to the development.

Reviewer 6:

The reviewer remarked that the corrugated electrodes structures with periodic grooves indeed just increase the overall porosity of the electrode. The reviewer said it is not going to help improve energy density at all and, in fact, the bad uniformity due to the periodic grooves may have significant negative effect on life.

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 replied that goals were achieved, adding that there was some discussion over fast charge, which is still to be completed.

Reviewer 2:

The reviewer found that project team was able to demonstrate electrodes with both power and energy-density performance. Challenges remain around lower initial capacity due to grooves that can take 10%-15% of the porosity.

Reviewer 3:

The reviewer indicated that the process has produced working electrodes that have some performance attributes worth considering. However, the cost projections are not terribly compelling at this stage, and there is no cost projection based strictly on the adoption of the process itself.

Reviewer 4:

The reviewer commented that the authors have been careful to track their process through pressing the electrode, ensuring their structure is maintained. The one area that was not focused on was the stability of the electrode around these depressions. The reviewer said there is a lack of discussion of the negative-to-positive (N:P) ratio around the depressions. It is likely that around these depressions there is a severe mismatch of the N:P ratio, which may cause lithium plating. This, combined with fast charging, should reduce life and potentially make this a technology that could not be used in a practical application. This is a critical component of this project that was not addressed. The reviewer concluded that the industrial partners on this project should be aware of this and this should have been investigated.

Reviewer 5:

The reviewer found that comparison with baselines is not fair enough and that life comparison with baselines are not reported or have been conducted.

Reviewer 6:

While the performance of the electrodes is good in some measures, the reviewer remarked that the porosity is too high. Cost reduction (greater than or equal to 30%) has not been demonstrated and the gravimetric performance improvements only meet the goal (20%) under a very limited (and generally unrealistic for EV or other real-world applications) circumstances—and actually become worse under likely usage scenarios.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer described collaboration as very clear on the roles and responsibilities, with evidence of contributions from all.

Reviewer 2:

The reviewer found good collaboration across team members.

Reviewer 3:
The reviewer said there was good collaboration with government and commercial entities and no issues noted.

Reviewer 4:
The reviewer stated that various relevant partners are involved in the project.

Reviewer 5:
The reviewer replied that it seems reasonable.

Reviewer 6:
There is a good list of partners, but the reviewer indicated that the previous question highlighted a problem the partners should have discussed and researched.

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 there is a good plan for future work in the limited time left on the project.

Reviewer 2:
The reviewer stated that the technical goals for next steps appear reasonable but that more detail of cost projections also needs to be developed.

Reviewer 3:
The reviewer said that life studies are in future research. Given that the project is nearing completion, it is unlikely that if life is poor it can be researched within the scope of this project. The reviewer added that there is a good opportunity for a follow-up project to this on optimization of these depressions for life.

Reviewer 4:
The reviewer responded this is N/A.

Reviewer 5:
The reviewer wrote that full-cell performance demonstration and scale-up is good. The reviewer is skeptical that fast charging will be improved with this electrode, since this performance is normally anode governed.

Reviewer 6:
The reviewer asserted it does not matter how big or small the cathode, the corrugated electrodes structures with periodic grooves indeed just increase the overall porosity of the electrode and are less likely to help improve energy density at all.

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

Reviewer 1:
The reviewer offered that finding ways to produce electrodes in a cheaper and better way is critical to achieving DOE goals.

Reviewer 2:
The reviewer said this approach improves cell performance, but with no appreciable cell-cost increase.

Reviewer 3:
The reviewer commented that cathode-production technology is a major cost driver in the overall cost of the Li-ion product line and exploring alternative techniques appears prudent.

Reviewer 4:
The reviewer wrote that cheaper, lighter batteries would lead to cheaper, better-performing EVs.

Reviewer 5:
It was s unclear to the reviewer if this is a fast charge or high-energy density project. The reviewer suggested that the authors could have benefited from their partners providing better metrics to calculate in a more meaningful way. While it still hits DOE objectives, this project is not categorized clearly.

Reviewer 6:
The reviewer remarked that the approach is not a right direction to support DOE objective: higher energy, lower cost.

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 no issues of excessive resources.

Reviewer 2:
The reviewer indicated that resources are sufficient.

Reviewer 3:
The reviewer wrote there are no issues.

Reviewer 4:
The reviewer replied that the project is ending.

Reviewer 5:
The reviewer could give no feedback because of being unclear about resource utilization.

Reviewer 6:
The reviewer remarked it was the wrong approach and could not achieve the stated milestones.

Presentation Number: bat272
Presentation Title: Prelithiation of High-Capacity Battery Electrodes
Principal Investigator: Yi Cui (SLAC National Accelerator Laboratory)

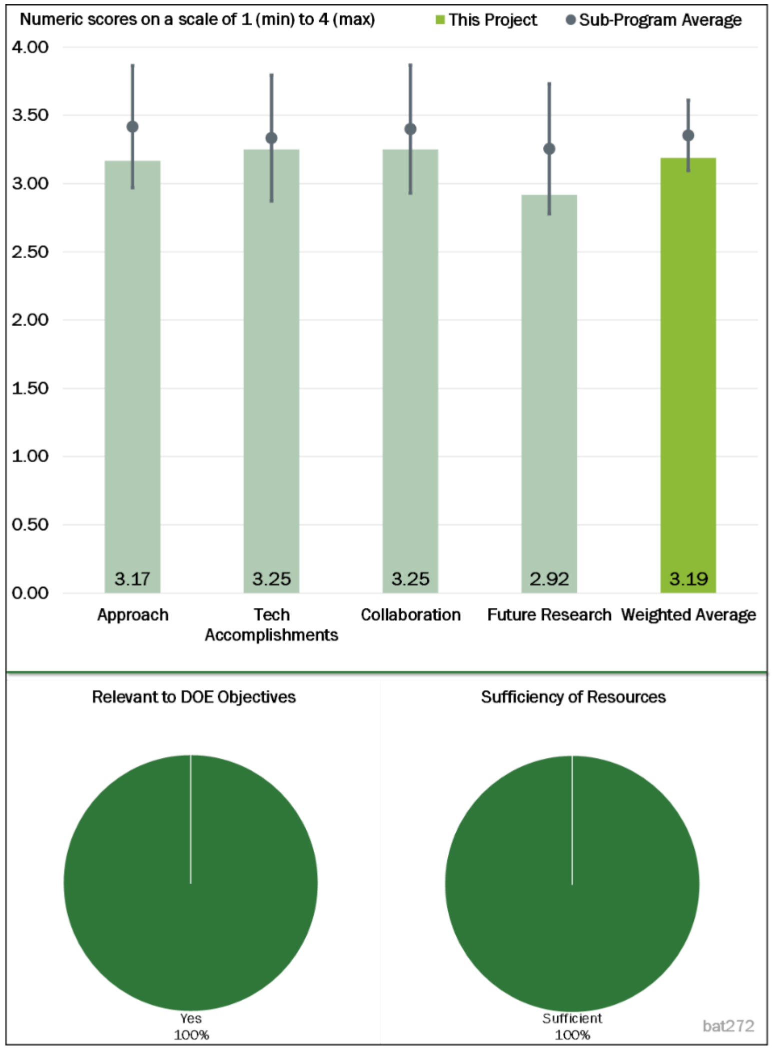

Figure 2-20 – Presentation Number: bat272 Presentation Title: Prelithiation of High-Capacity Battery Electrodes Principal Investigator: Yi Cui (SLAC National Accelerator Laboratory)

Presenter

Yi Cui, SLAC National Accelerator 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 that the performer has proposed a variety of innovative methods to pre-lithiate the anode or cathode, which should improve the first cycle CE.

Reviewer 2:

The reviewer stated that the PI has developed a few approaches to pre-lithiate anodes and cathodes, adding that the approaches are feasible and effective.

Reviewer 3:

The reviewer called the work beautiful, but said that pre-lithiated Si and SiO_x are common among battery suppliers.

Reviewer 4:

The reviewer indicated that the work is aimed at pre-lithiation methods and reagents in both the anode and cathode with focus on stability of reagents during manufacturing processes. The reviewer described this as a practical effort to improve efficiency and energy density of Li batteries. Many technical approaches are apparently under study. The reviewer added that there is some lack of clarity on prioritization and focus.

Reviewer 5:

The reviewer stated that numerous interesting approaches and materials strategies were presented for pre-lithiation of both anode and cathode materials (some of them going back to 2011, well before the project started). However, the reviewer observed, it seems this work is more focused on the initiation of new materials concepts than on following through and solving all of the challenges needed to actually achieve pre-lithiation. The reviewer suggested the approach would likely be more effective if the project team chose just one or two concepts and attempted to carry them through to completion.

Reviewer 6:
The reviewer stated that the researcher has demonstrated several techniques for pre-lithiating anode materials and cathodes over the past 5 years. For 2018 the PI focused on pre-lithiating Group 4 elements. The reviewer added that while these techniques lead to better performance, there is very little explanation behind the improvements.

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 number of approaches have been demonstrated to pre-lithiate Si anodes with good air stability and NMP compatibility. The reviewer also noted that lithium fluoride (LiF), lithium oxide (Li_2O), Li_2S, and lithium nitride (Li_3N) were also used to develop pre-lithiated cathodes. The reviewer found that the electrodes demonstrate excellent electrochemical performance.

Reviewer 2:
The reviewer explained that the performer demonstrated improved first-cycle CE using lithium-silicon compounds (Li_xSi) or alloyed lithium-silicon dioxide (Li-SiO_2) anode pre-lithiation. The reviewer elaborated that cathode pre-lithiation was generally effective in improving first-cycle CE, but the project team needs to quantify the impact on energy density from the residual pre-lithiating agents. The reviewer added that free standing air-stable Li-graphene foil can be an effective method to pre-lithiate the anode. Additionally, the molten lithium pre-lithiation approach might be difficult to implement for large-scale manufacturing.

Reviewer 3:
The reviewer indicated that numerous interesting materials strategies are presented, and some promising results are shown. However, it was hard for the reviewer to tell exactly what has been accomplished against the key metrics for pre-lithiation, which include cell performance and manufacturing aspects. A clear set of metrics and progress against all of the metrics would be very helpful.

Reviewer 4:
The reviewer stated that the principal investigator has demonstrated several methodologies for pre-lithiation of the cathode and the anode over the past 5 years. For this review, the reviewer only focused on those efforts published in 2018, which is the pre-lithiations of Group 4 elements that are partially oxidized. The reviewer explained that these materials are submersed in Li-metal and transformed to fully alloyed metals and Li_2O. The materials that start with some oxide cycle better than those without oxide. No explanation is provided that is substantiated by follow-up experiments.

Reviewer 5:
A reviewer noted that a comprehensive and dynamic presentation of extensive PI work on pre-lithiation dating back to 2011 was shown. The reviewer offered that the PI seems to be the world's leading expert on novel pre-lithiation R&D with prolific publications in high impact journals. However, the reviewer noted, most, if not all, of the slides presented are from work prior to this program, including five slides entirely with materials previously presented during Annual Merit Review (AMR) review of the predecessor program. The reviewer concluded that it is difficult to be clear on what specifically has been accomplished in the program starting in August 2017. Particularly, there is a lack of clarity on work accomplished over the last year.

Reviewer 6:
The reviewer asserted that the fact that the process cannot use a water-soluble binder will inhibit industrial application.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted the performer has identified an industrial partner, Amprius, for technology transition, and added that the performer also effectively leveraged the X-ray capability at SLAC to characterize the samples.

Reviewer 2:
The reviewer replied that the PI collaborates some with a researcher at SLAC for X-ray data and another professor at Stanford who tries to develop new ways to stop Li dendrites.

Reviewer 3:
The reviewer stated that collaboration with key partners is listed.

Reviewer 4:
The reviewer found appropriate collaboration.

Reviewer 5:
The reviewer said the PI is collaborating with SLAC for X-ray characterizations but suggested more partners across the program.

Reviewer 6:
The reviewer observed that collaborations with SLAC, Amprius, and Professor Bao are all mentioned, but that it is a little difficult from the presentation to tell how substantial these are.

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

Reviewer 1:
The reviewer agreed with the proposed focus on manufacturing processes and electrode-level development.

Reviewer 2:
The reviewer found wonderful new ideas, but no approach yet to deal with water versus NMP.

Reviewer 3:
The reviewer commented that the PI proposed to demonstrate an anode pre-lithiation process to be compatible with a variety of solvent processing. The reviewer described the proposed research as appropriate and important for further utilization of the pre-lithiated electrodes. The PI included pouch cell testing in the approach slides but provided no results about the pouch cell test.

Reviewer 4:
The reviewer said the performer should demonstrate the pre-lithiation techniques in full cells using practical N:P ratios and loadings.

Reviewer 5:
The reviewer noted that the research proposes to continue to try to find effective ways to make stable, pre-lithiated anode and cathode materials. Also, the research would like to look into pre-lithiating electrodes. However, the reviewer stated that no details are provided.

Reviewer 6:
The reviewer remarked that the future work statement is very activity oriented but without metrics. It is focused on understanding, exploring, and synthesizing. The reviewer asked what critical gaps remain, and how the project is specifically addressing them.

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

Reviewer 1:
The reviewer replied that developing a low-cost and manufacturable pre-lithiation technique is critical for high-energy density cells with Si anode.

Reviewer 2:
The reviewer commented that this project is aimed at development of pre-lithiation reagents and methods to improve first-cycle efficiency and battery energy density contributing to the development of higher energy density batteries, a key DOE objective.

Reviewer 3:
The reviewer responded that the topic and the research certainly are relevant to DOE objectives, as they are focused on improving pre-lithiation for Li-battery electrodes. The reviewer suggested that some of the approaches here, if carried through and extended on, may be helpful to the accomplishment of pre-lithiation in a practical cell.

Reviewer 4:
The reviewer stated that first-cycle inefficiency can take away from cell energy density, so improving on this through a low-cost method further helps DOE meet its specific energy targets.

Reviewer 5:
The reviewer wrote that many of the high-capacity electrodes suffer from low CE and, therefore, pre-lithiating the electrodes helps to address this issue and enable a high-energy cell for vehicle applications.

Reviewer 6:
The reviewer said it was appropriate.

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 with the amount of resources, the performer has developed an extensive, innovative portfolio of pre-lithiations for the anode or cathode.

Reviewer 2:
The reviewer said the team has enough resources to try several approaches and several modifications to the casting process.

Reviewer 3:
The reviewer found the resources are sufficient to complete the project.

Reviewer 4:
The reviewer replied there is no evidence of insufficient resources.

Reviewer 5:
The reviewer wrote that the listed milestones are not quantitative but more activity based; however, resources are adequate for such an endeavor.

Reviewer 6:
The reviewer replied okay.

Presentation Number: bat275
Presentation Title: Lithium Dendrite Prevention for Lithium Batteries
Principal Investigator: Wu Xu (Pacific Northwest National Laboratory)

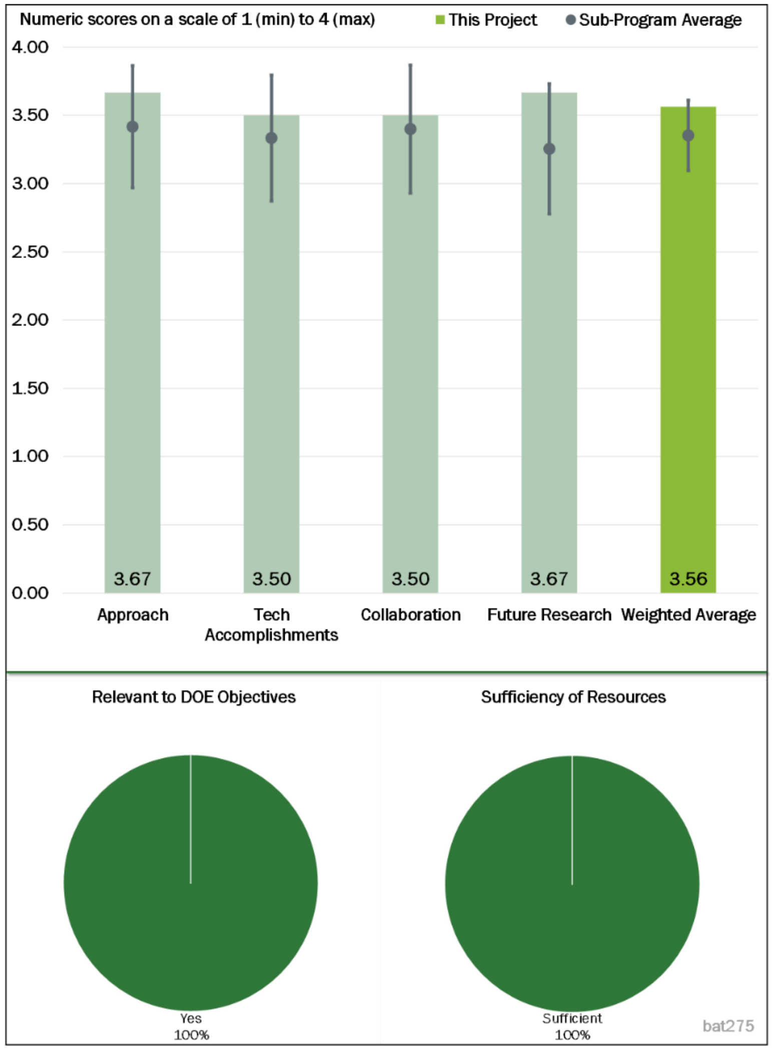

Figure 2-21 – Presentation Number: bat275 Presentation Title: Lithium Dendrite Prevention for Lithium Batteries Principal Investigator: Wu Xu (Pacific Northwest National Laboratory)

Presenter

Wu Xu, 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 explained that in the project, PNNL focused on developing new electrolytes (high-concentration electrolytes and hybrid polymeric-composite electrolytes) to solve the issues of Li dendrites growth, low CE and low-charge current density. The reviewer elaborated that electrolytes are the key component determining Li-deposition behavior and c CE. PNNL's work successfully uses high-concentration electrolytes with commercially available chemicals to regulate Li growth, eliminate Li dendrite growth, and increase CE to 99.3%. Their systematical investigation on different types of electrolytes (carbonate based, alkyl phosphate based, ether based, and polymer based) is well designed and provides profound understanding for future electrolyte design. Although further study on Li-metal anodes still needs to be performed, their results have made very good progress. Therefore, the reviewer concluded that the team's approach to perform the work is excellent.

Reviewer 2:

The reviewer stated that in this project, high-concentration electrolytes (HCEs), polymers in "quasi-ionic liquid" electrolytes (PQILEs), and solid-state polymer-in-salt electrolytes have been demonstrated to be effective in overcoming barriers for Li-metal anodes, such as low CE, Li dendrite formation, and unstable cyclic performance. The reviewer found these approaches are very well designed and very important for solving the critical problems of Li-metal anodes.

Reviewer 3:

The reviewer said the approach applied a hybrid polymeric composite electrolyte to protect Li-metal anodes and minimize the dendrite formation, adding that the objective is clear.

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 indicated that the PI made significant accomplishments in all three areas listed in the Technical Approach and the project milestones have been completed according to the project plan. CE over 99% with granular and compact Li deposition was achieved by an inorganic and polymer hybrid composite electrolyte. The most impressive result is that Li NMC-333 cell with polymers in "quasi-ionic liquid" electrolytes (PQILEs) delivered stable cyclic performance and good rate capability at both around room temperature and high temperature with a cut-off voltage up to 4.4V.

Reviewer 2:

In terms of the technical accomplishments and progress toward overall project, the reviewer responded that the milestones have been reached. Additionally, results collected under well-designed experiments have fully illustrated the effects of different high-concentration electrolyte and polymers on Li deposition morphology and CE. The reviewer said that the progress toward overall project is effective. PNNL has collected very good results, which not only contribute to the understanding of different electrolyte systems, but also to overcoming the barriers of the Li-metal anode.

Reviewer 3:

A reviewer replied that a highly stable cell has been demonstrated with hybrid polymer-in-salt composite electrolytes and NCM-333. It can be cycled for hundred cycles up to 4.4V.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted that in the project, PNNL collaborated with ANL and U.S. Army Research Laboratory to do the work, adding that all of them have participated in the project and are very well coordinated. Furthermore, all of them have contributed to the project and did a very good job.

Reviewer 2:

This reviewer stated that this project has a very good team and good collaboration with ANL and the U.S. Army Research Laboratory.

Reviewer 3:

The reviewer had no comment.

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 development of hybrid polymer-in-salt composite electrolytes and the evaluation in Li-metal batteries are the key to the success of this project.

Reviewer 2:

The reviewer explained that for future work, PNNL proposed two directions. One is to continue their original study on hybrid polymer-in-salt composite electrolyte. The other one is to study the impacts of solid polymer electrolyte on Li deposition morphology and CE. Besides, the project team also proposed the target for Li-NMC-532 full cells. Generally speaking, the reviewer said, based on their previous work approach and the results that have been collected, the future research plan the project team proposed follows their previous research and is feasible as well as effective to overcome the barrier.

Reviewer 3:
The reviewer found future work plans for this project are well identified. This project is proposing to optimize hybrid polymer-in-salt and solid-state polymer-in-salt electrolytes to achieve stable cyclic performance for 4V Li||NMC-532. More efforts are needed for increasing the CE of Li-metal anode.

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

Reviewer 1:
The reviewer said yes, explaining that this project aims to overcome the critical challenges of the Li-metal anode, which is very important to achieve a Li rechargeable battery with high energy density and long cycle life. This is directly related to DOE goals.

Reviewer 2:
The reviewer said the project supports the overall DOE objectives. This project, focusing on investigating effects of different electrolytes on Li deposition morphology and CE, has achieved good results in eliminating Li dendrite growth and increasing Li plating and striping CE to as high as 99.3%. Moreover, the reviewer noted, the project team's systematic study on different electrolytes system provides understanding and guidance for electrolyte-system design.

Reviewer 3:
The reviewer agreed that it has important approaches to addressing solid-state 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 replied that the stated milestones have been achieved in a timely fashion. Various electrolytes have been evaluated thoroughly and the resources for the project have been used very sufficiently.

Reviewer 2:
The reviewer said the team has adequate resources to carry out the proposed work.

Reviewer 3:
The reviewer had no comment.

Presentation Number: bat276
Presentation Title: Mechanical Properties at the Protected Lithium Interface
Principal Investigator: Nancy Dudney (Oak Ridge National Laboratory)

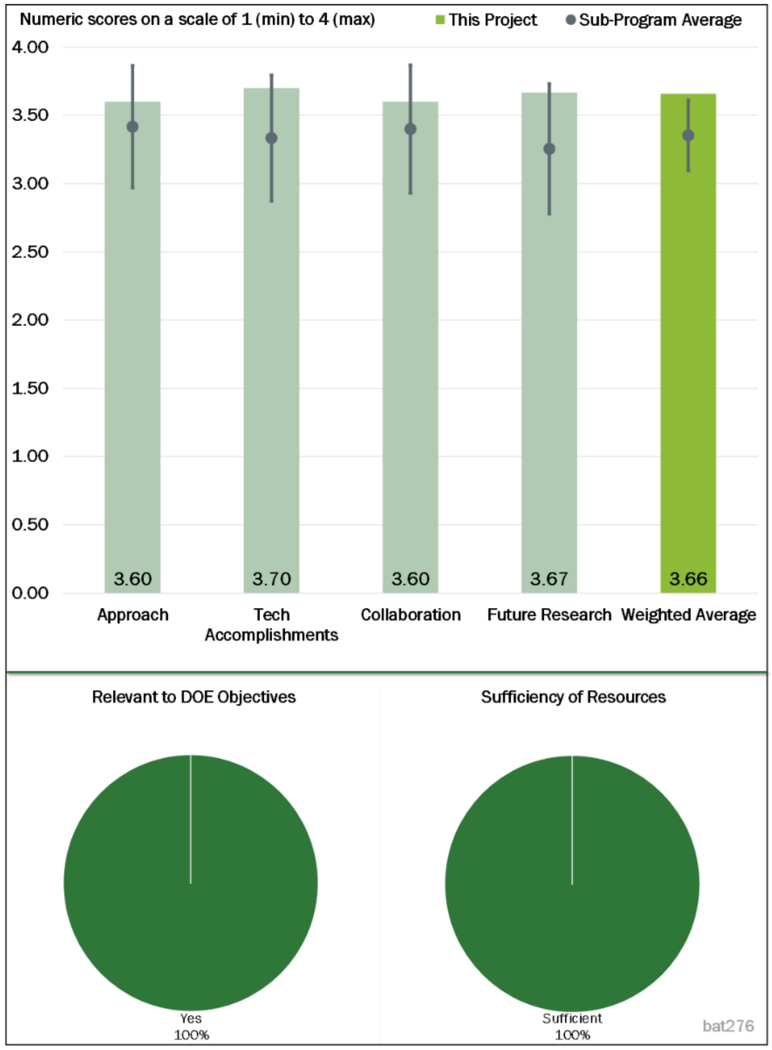

Figure 2-22 – Presentation Number: bat276 Presentation Title: Mechanical Properties at the Protected Lithium Interface Principal Investigator: Nancy Dudney (Oak Ridge National Laboratory)

Presenter
Nancy Dudney, 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 praised the project as outstanding and important work, elaborating that it is foundational for understanding and overcoming challenges with dendrites. The reviewer further praised the quality and insights from this work as exceptional. The reviewer has read the Herbert and Dudney papers, and they provide important property measurements and insights that truly contribute to advancing the understanding of Li dendrites.

Reviewer 2:
The reviewer stated that the project team has shown that the multiscale mechanical measurement tools (nano-indentation to macro-scale tensile and adhesion) can be very useful to understanding Li-metal electrodes and solid-state electrolytes.

Reviewer 3:
The reviewer commented that the PI developed multiple methods to study the mechanical properties of the solid electrolyte, thin Li anode, and their buried interfaces. The reviewer found the project is well designed and helped to understand the mechanical behavior of Li/ and the solid electrolyte interface during cycling with and without pressure.

Reviewer 4:
The reviewer wrote that studying the difference between Li foil-SSE versus vapor deposited Li-SSE interface is an effective approach to gain insights on the Li-SSE interface.

Reviewer 5:

The reviewer explained that the team has probed the mechanical properties of Li-metal and solid electrolytes to understand the stress and relaxation and map out controlling mechanisms at the interface of Li to understand Li dendrite formation. Their approach was to come at the mechanism at two lengths scales. The reviewer found that the team's results were unique by showing the relationship between the adhesion strength and area-specific impedance (ASI) of the LLZO pellet and Li-metal. Additionally, the reviewer noted, with nano-indentation, the project team was able to show yield stresses and, from the work, hypothesize why Li dendrite formation occurs. While the work is unique and the correlations shown are important, it would be good to study real cells. Also, it would be interesting to the reviewer to investigate the mechanical properties after several cycles. The reviewer wondered if changing the Li thickness matters.

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 praised the publications and insights from this project as outstanding, adding that measurement of these properties has been long overdue, and the measurements are providing important insights.

Reviewer 2:

The reviewer concluded that the project team has made great progress over the funding period. It is good to show the pressure-dependent current density for void-free Li stripping. The mechanical property of Li with different volumes also helps to understand the interface. It is also shown that grain boundaries also show great mechanical strength. The reviewer wrote that all of these accomplishments help to understand the mechanical behavior of Li SEIs.

Reviewer 3:

The reviewer wrote that the project provided valuable insights on the Li-SSE interface. The reviewer explained that the project team found that small amounts of Li in confined space (e.g., Li dendrites) had a higher modulus than bulk Li. The project team also found unexpected creep in glassy SSE. These insights should guide the design of the Li-SSE interface to mitigate Li dendrites.

Reviewer 4:

The reviewer replied that main goals of the project were in understanding what happens at the Li-SEI, adding that the project team was able to study in ideal situations the correlation between the critical stack loading to the current density. The project team has also studied the interface resistance and adhesion strength of the LI and the solid-state electrolyte interface. All these mechanical properties are great under ideal conditions. However, the reviewer said, it would be great to have seen how these mechanical properties change under non-ideal conditions.

Reviewer 5:

The reviewer noted the project is 100% complete with a large number of publications and presentations.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Clearly, the reviewer remarked, this was an outstanding collaboration among Nancy Dudney and Eric Herbert, in particular, with Jeff Sakamoto also playing a key contributing role. The reviewer said there is no question this project team worked together well.

Reviewer 2:

The reviewer found a strong project team with strong university and equipment suppliers participating.

Reviewer 3:
The reviewer said the project team demonstrated effective collaboration by partnering with others to quantify stress at the Li-SSE interface.

Reviewer 4:
The reviewer agreed that the project team used the collaborations well.

Reviewer 5:
The reviewer said this project involves collaborations between National Laboratories and several universities.

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 wrote that, unfortunately, the project is over, but the next steps identified are all well informed and will contribute to further progress (e.g., moving to full cells, etc.)

Reviewer 2:
The reviewer noted the project has ended.

Reviewer 3:
The reviewer stated the project has ended.

Reviewer 4:
The reviewer indicated that the project is completed.

Reviewer 5:
The reviewer remarked that the proposed future research is not sufficiently detailed for this reviewer to evaluate.

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

Reviewer 1:
The reviewer said this project is providing critically important measurements to understand Li plating stability, directly contributing to DOE goals.

Reviewer 2:
The reviewer wrote that understanding the mechanical properties of the Li-solid state interface is important for developing an all solid-state battery. This work on understanding the stress-and-strain relationships are an important step into creating better systems.

Reviewer 3:
The reviewer found that understanding of the mechanical behavior of components in all solid-state batteries is shown by the project team and others to be very important to reach the goals of energy density (500-700 Wh/kg) and cycle life (3,000-5,000 deep- discharge cycles).

Reviewer 4:
The reviewer replied that employing Li anode with solid electrolytes can potentially improve the safety and energy density of batteries.

Reviewer 5:
Understanding the Li-SSE interface is key to mitigate Li dendrites.

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 this team has gotten A LOT done with the resources they have. Unfortunately, the reviewer wrote, the project is now ending.

Reviewer 2:
The reviewer said the team has ample resources.

Reviewer 3:
The reviewer found the resources were reasonable and appropriate.

Reviewer 4:
The reviewer said the funding was sufficient for the proposed tasks.

Reviewer 5:
The reviewer remarked that the work done here has been sufficient and provides good insight into the surface properties of Li metal and the interface stress and strains. It would be good to have seen results under non-ideal conditions to see how these results change. For example, the reviewer wanted to know what the results are after one cycle versus pristine. The reviewer questioned if this is a good technique to use to understand what is happening before dendrite formation.

Presentation Number: bat280
Presentation Title: Novel Chemistry: Lithium-Selenium and Selenium-Sulfur Couple
Principal Investigator: Khalil Amine (Argonne National Laboratory)

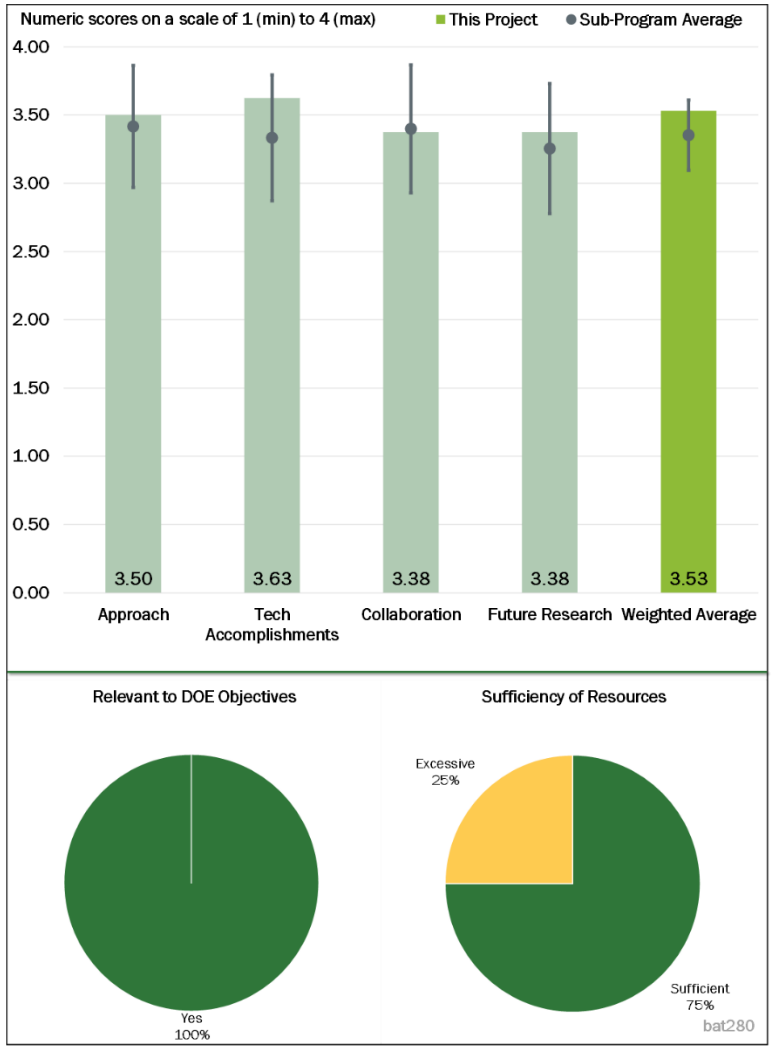

Figure 2-23 – Presentation Number: bat280 Presentation Title: Novel Chemistry: Lithium-Selenium and Selenium-Sulfur Couple Principal Investigator: Khalil Amine (Argonne National Laboratory)

Presenter
Khalil Amine, Argonne National Laboratory

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

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

Reviewer 1:
The reviewer praised the approach as an excellent and well-planned one to develop novel Sulfur and Selenium composite (S_xSe_y) cathode materials for high-energy-density Li batteries with low cost and high safety.

Reviewer 2:
The reviewer commented that the PI and the project team have developed a unique electrochemistry storage chemistry of a Se- and S-based cathode and Li-metal anode. The reviewer offered that the new Li-Se/S system promises very high energy-storage capacity. The project team is further exploring new electrolytes in order to improve this new Li-Se/S in this review period. The approach is highly innovative.

Reviewer 3:
The reviewer said the approaches adopted by the project, using macro-porous carbon for high Se-S loading and the novel concentrated siloxane-based electrolyte to enable shuttle-less cycling, have significantly improved the performance of the Li/Se-S battery.

Reviewer 4:
The reviewer indicated that there were several parts to the approach: The first was to examine high-loading the S-Se cathode on microporous carbons of different pore size and volume porosity, and high load S-Se in the cathode material to increase volumetric energy density using a fluorinated ether-based electrolyte. Another step was to explore concentrated siloxane-based electrolytes to suppress the polysulfides and polyselenides shuttle. The third part was to understand the effect of concentrated siloxane-based electrolytes on Se-S cathode chemistry using multiple diagnostic tools. High loadings of the cathode have been demonstrated, which

showed reasonably good performance in fluorinated ether or concentrated siloxane solutions. It was shown using in situ XRD that there is not any formation of Li_2S in concentrated siloxane solutions.

These results are encouraging, but some of the questions the reviewer wanted to know what the composition of the concentrated electrolytes is, whether these cycling data are at room temperature, and what the loading is of the cathode, even with heavily loaded sulfur in carbon (70-85%).The reviewer noted that if the active material loading is low (i.e., low mg S/cm^2 or mAh/cm^2), this performance does not mean much or is even misleading.

The reviewer wrote that hopefully these will be addressed in the future studies, including the amount of Se needed in S to make any impact on conductivity or PS effects. Comparative studies with Li-S cells in the same conditions need to be made to understand the benefits of Se in S cathodes. The reviewer concluded that the project is well integrated with the other VTO 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 remarked that the highly accurate leakage-current-measurement system developed by the project team has been used to confirm the shuttle-less electrochemical cycling. The new electrolyte makes it possible to develop high performance with long cycling life. It is a very impressive achievement.

Reviewer 2:

The reviewer agreed that the team has made a significant progress, elaborating that it used macro-porous carbon to host high Se-S loading in the cathode materials to increase volumetric energy density, and novel concentrated siloxane-based electrolytes were developed to suppress polysulfides and polyselenides shuttle. The project team also investigated the function mechanism of concentrated siloxane-based electrolytes on the solid-solid lithiation chemistry of the cathode using multiple diagnostic tools.

Reviewer 3:

The reviewer found that the team has made significant progress and met and is on track to meet all the required milestones in this review period. In this review period, the reviewer explained, the team has focused on electrode optimization and application of a novel concentrated siloxane-based electrolyte to suppress the polysulfides and polyselenides dissolution effect. The project team has used electrochemical characterization to demonstrate the improved performance, and used synchronized-based X-ray diffraction and the X-ray absorption near-edge structure (XANES) method to demonstrate that polysulfides and polyselenides do not dissolved in the siloxane-based electrolyte, and use ab-initio molecules dynamic simulation to confirm theoretical non-interaction between the electrolytes, polysulfides, and polyselenides.

Reviewer 4:

The reviewer responded that reasonably good progress has been made in demonstrating high specific capacity and good life, especially in concentrated siloxane electrolytes. However, there is no baseline, i.e., Li-S cells (and also Li-Se cells) with same porous carbon hosts and siloxane electrolytes to quantitatively ascertain the benefits of Se-blending with S. The reviewer said the results are not as convincing without the details on the concentrated siloxane solutions (its conductivity at room and low temperatures, for instance) and without high active material loading in the cathode. It appeared to the reviewer that the area-specific capacity mAh/cm^2 is not high and it is more challenging to get good cycle life with high areal capacities. The reviewer also noted that CE is incorrectly represented here; the reviewer asserted that it is discharge capacity over charge capacity and is less than 100% for Li-S due to the PS shuttle. Similarly, it was not clear to the reviewer how leakage or self-discharge current can be correlated with shuttle effects. In situ XRD probing is useful, especially if performed on dense electrodes. Overall, though, the reviewer said the progress achieved here is meaningful and relevant to the DOE goals.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer noted that the project team collaborated extensively with the University of Maryland and Western University and within ANL's Advanced Photon Source (APS) and theory group. A lot of technical accomplishments came out of the collaborations.

Reviewer 2:

The reviewer said the PI has good collaborations with University of Maryland, ANL, and Western University.

Reviewer 3:

The reviewer replied that the project team and partners include a National Laboratory and universities with strong expertise in materials synthesis and characterization.

Reviewer 4:

The reviewer found that there are good collaborations with several researchers within DOE Laboratories and with universities, especially in performing in situ studies and ab-initio molecular dynamic simulations. Collaboration efforts for the surface coating have not begun yet.

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 PI has proposed very relevant future work for FY 2020, centered on increased active materials loading and Li-electrode behaviors.

Reviewer 2:

Writing that the proposed work is both logical and necessary to move forward, the reviewer indicated that the project team will further understand the interfacial chemistry of cathode and electrolyte and develop the high-loading cathode. More important, the Li-metal anode issues are also planned to be addressed.

Reviewer 3:

The reviewer said that the FY 2019 milestones (quarter [Q] 2 and Q3) are critical steps to ensure high performance of a full battery. With the shuttle-less electrolyte, it is promising to develop effective protective layers for the Li-metal anode.

Reviewer 4:

The reviewer commented that future studies to examine cathodes with high areal loading, to understand the cathode-electrolyte interface, and to stabilize the Li-metal anode are appropriate and logical. The reviewer wrote it would be better to demonstrate the benefits of $S_{22}Se$ cathode in comparison with S cathode with the same microporous carbons and electrolytes and also demonstrate in a pouch cell of reasonable size and without excess electrolyte.

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

Reviewer 1:

The reviewer agreed the project is highly relevant and supports DOE objectives, because it aims to develop high-energy- density and long-life Li-metal batteries with low cost and high safety.

Reviewer 2:
The reviewer affirmed that developing new electrochemical couples for high-energy-density Li-based rechargeable cell is very relevant to DOE's objective. The reviewer said this project investigates new chemistry that can lead to a high-energy-density battery.

Reviewer 3:
The reviewer remarked that Li-S or Li/Se-S batteries are low-cost solutions for large-scale energy storage, and that the project aims to improve the performance by increasing energy density (600 Wh/kg) and cycling life (500 cycles).

Reviewer 4:
For a widespread use of EVs and plug-in hybrid electric vehicles (PHEVs), the reviewer commented, batteries with higher energy and lower cost than the current Li-ion batteries are needed and Li-S system is expected to fulfil these needs because of the high capacity and low cost of S. New, high-capacity and long-life sulfur cathode materials (with necessary modifications) are desired to meet the DOE goals, which this project has been 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 found that it is a strong team led by a National Laboratory and supported by university partners. The synchrotron X-ray facility and the lab developed novel equipment (leakage current detector), which played great roles in conducting the project.

Reviewer 2:
The reviewer found that there are sufficient resources for the project to achieve the stated milestones in a timely fashion.

Reviewer 3:
The reviewer replied that the resources are sufficient for making timely progress.

Reviewer 4:
The reviewer indicated the resources are a little excessive for the scope of the project as well the progress accomplished.

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

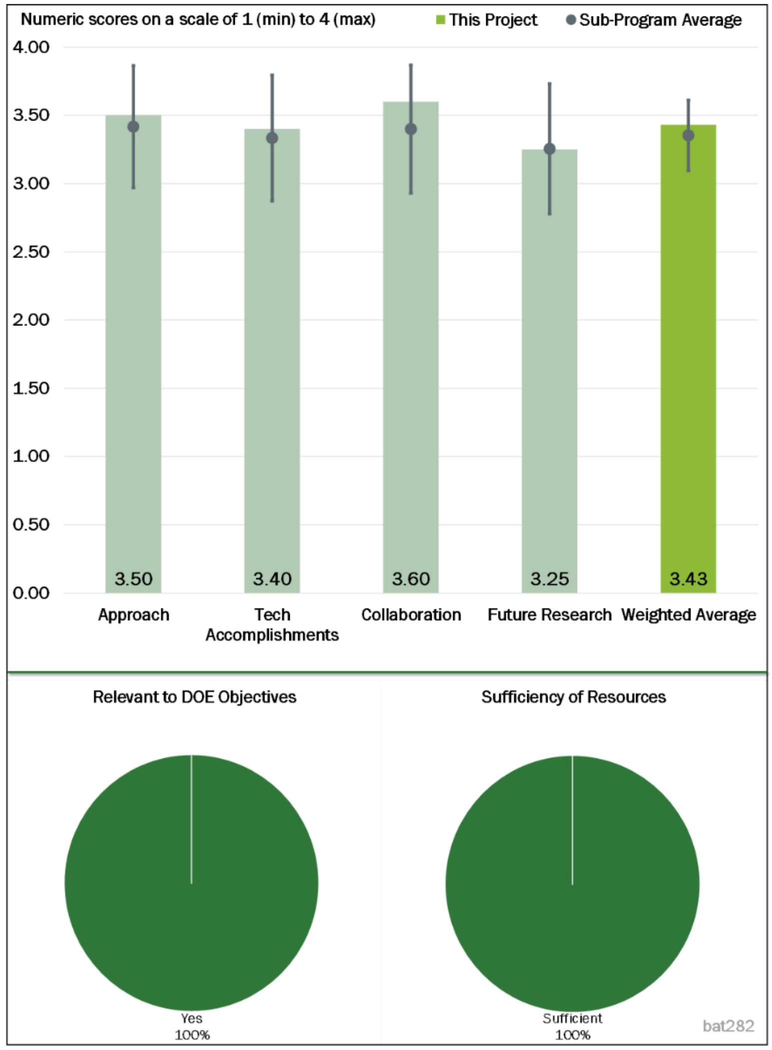

Figure 2-24 – Presentation Number: bat282 Presentation Title: Development of High-Energy Lithium-Sulfur Batteries Principal Investigator: Dongping Lu (Pacific Northwest National Laboratory)

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:

This reviewer found that the project takes an excellent approach in the investigation of a Li-S battery, adding that the project focuses on the S electrode to improve its ionic conductivities, to decrease porosity, and to limit the electrolyte usage. These are all very important aspects to be investigated to enable a Li-S battery.

Reviewer 2:

The reviewer explained that the objective here is to understand the life-limiting properties of Li-S cells with a heavily loaded S cathode in lean-electrolyte conditions and to develop low-porosity S cathodes for improving energy density. Overall, the reviewer elaborated, the efforts address the barriers of low practical energy density, shuttle effect, low rate capability, and limited cycling of Li-S cells. The approach is to design a test cell for the hybrid electrolyte study, identify life-limiting factors of Li-S cells, develop composite S cathodes with a sulfide solid electrolyte, and a develop low-porosity electrode by dry processing to function with low electrolyte content. Additionally, functional coatings over a Celgard separator were examined for reducing PS shuttle. Finally, a highly conducting solid electrolyte based on mixed halide-substituted sulfides, i.e., $Li_7P_2S_8Br_{0.5}I_{0.5}$, was developed.

It was not clear to the reviewer what additional data were generated with the hybrid cell (apart from the wetting characterization) and what cell was used for the subsequent cycle-life data with sulfur cathodes of different thickness and with different electrolyte amounts. The reviewer asked if the 350 Wh/kg pouch cell described later has been at all for any of these studies, especially to understand the effects of S loading and electrolyte content and to test the dense cathode. The reviewer wanted to know whether the solid electrolyte-blended sulfur cathode has been tested. Even though these individual aspects seem to be meritorious, the overall approach seems to be a bit disconnected and not so much focused on the overall objective of high-specific-energy, energy density Li-S cells.

Nevertheless, the reviewer concluded that the project is well oriented to demonstrate the improvements toward high-energy and low-cost Li-S cells, consistent with the goals of DOE's Vehicle Technologies program. The project is also well integrated with the other VTO projects.

Reviewer 3:

The reviewer said that novel electrolyte cell with garnet oxide membrane provides a reliable way to characterize the reaction mechanism of a Li-S battery under various conditions, such as different S loadings, N:P electrode ratios, and electrolyte-sulfur (E-S) ratio.

Reviewer 4:

The reviewer found that it is a reasonable approach to develop a high-energy Li-S battery using a hybrid electrolyte, i.e., a solid electrolyte in the middle can be used to prevent the shuttle effect and liquid electrolyte in the cathode can be used to improve the interfacial contact.

Reviewer 5:

To achieve the high-energy Li-S batteries, the reviewer indicated that many key barriers need to be solved first, such as high S loading, low E-S ratio, and the shuttle effects of polysulfides. In this project, the PI has proposed effective approaches to solve these barriers very well. For example, the project team has achieved S/Li-ion (Li^+) conductor cathodes with sulfur mass loading greater than 4 mg/cm^2 and S more than70 wt. % in the whole electrode and cycled at low E-S ratio (E-S less than 3 microliters per milligram [µL/mg]). The reviewer concluded that the approach proposed by the PI has addressed the technical barriers in some extent and the project is well designed and feasible.

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 concluded that the project team achieved excellent technical accomplishment during this review period. The project team also achieved milestones on time and on track to accomplish all the required milestone for the remaining time of this fiscal year. The reviewer said that the project team designed and made a test cell, which decoupled the interferences of Li counter electrode. This approach allows studying S electrode with the interferences of the counter electrode. The team quantified the effect of the electrolyte on the S electrode performance and demonstrated electrolyte content has a large impact to the cell performance. The reviewer said the team investigated the functional separator electrode as suggested by a reviewer. Finally, the reviewer noted that the team investigated the Li-sulfide, high ionic conductivity materials.

Reviewer 2:

The reviewer explained that the PI has focused on developing high-energy Li-S cells at practical S loading and low E-S ratio. The project team has proposed to prepare a highly conductive and low-porosity S cathode. The project team has developed high Li^+ conductivity S cathodes with room temperature conductivity greater than 1 mS/cm and low-porosity sulfur electrodes (electrode density greater than1 g/cm^3). By using these materials, the project team has achieved the relatively stable cycling of Li-S batteries at high S loading (at sulfur loading greater than 4 mg/cm^2 and greater than 6 mg/cm^2) and low E-S ratio (E-S less than 3 µL/mg). Therefore, the reviewer concluded, the technical accomplishments and progress are excellent.

Reviewer 3:

The reviewer found that reasonably good progress has been made overall. Specifically, the solid electrolyte-liquid electrolyte hybrid cell was designed but used only to understand the slow wetting process of the S cathode. The performance of Li-S was studied (not sure what the cell was) with different cathode loading, electrolyte amount, and Li thickness, which led to the (known) conclusion that lean electrolyte amount is a dominant factor. A low-temperature phase solid electrolyte $Li_7P_2S_8Br_{0.5}I_{0.5}$ with a high conductivity of 4.7 mS/cm was synthesized for making a composite S cathode. Furthermore, a dry-processing approach was developed for a high-loading and low-porosity S cathode preparation, which showed good performance with low electrolyte (again the reviewer asked what the cell used and what the cycling conditions are for this and for the studies with different cathodes and electrolyte contents). The reviewer inquired about what the failure mode is in these cells (only 40 cycles were shown in many cases), and if this dense cathode is blended with the solid electrolyte. The reviewer asked if there is a risk of cell shorting if the separator is coated with electronically conducting materials (carbon nanotubes [CNT], what are P1 and P2) on both sides. Overall, the reviewer concluded, the progress achieved here is meaningful and relevant to the DOE goals.

Reviewer 4:
The reviewer noted that PI has developed a sulfide solid electrolyte with a high ionic conductivity of approximately 10^{-3} S/cm. Incorporating a high conductive electrolyte in the cathode composite will help to increase the content of the S in the composite electrode. A dry-processing method was also demonstrated to prepare S cathodes with practically high loading, high-S content and high calendering density.

Reviewer 5:
The reviewer replied that the team identified the roles of N:P and E-S ratio in controlling the cycle life of the Li-S cell, a central problem in a Li-S battery. The separator coating and the new solid electrolyte enable long-term cycling stability.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
For the accomplishments and progress, the reviewer thought the project team has outstanding collaboration and coordination across the project.

Reviewer 2:
The reviewer noted that collaborators include National Laboratories, a university, and industrial companies, adding that the roles of each partner are clearly specified.

Reviewer 3:
The reviewer replied that the PI works with several partners including Brookhaven National Laboratory (BNL), University of Wisconsin–Milwaukee, and General Motors (GM). The PI also brought in another industry partner, Chemours Company, to address a reviewer’s request to investigate separators.

Reviewer 4:
The reviewer found that there are good on-going collaborations here within the DOE National Laboratories, e.g., BNL for reaction mechanism study, PNNL for materials characterization and electrochemical in situ study, and external collaborators, i.e., with General Motors on materials and electrode testing, the Chemours Company for the separator development, and the University of Wisconsin–Milwaukee for electrolyte and additive study. However, the reviewer indicated that it looks like nothing yet has been done on the electrolyte.

Reviewer 5:
The reviewer said the PI is collaborating with BNL, GM, and University of Wisconsin–Milwaukee on this project.

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

Reviewer 1:
The reviewer explained that although the PI has proposed many effective approaches and realized the cycling of Li-S cells at high S loading and low E-S ratio, the high energy Li-S batteries are still far away from practical application. So, the PI has proposed some very important key issues to be solved in the future research, such as

low S utilization rate of high-loading and low-porosity S electrodes, long-term cycling stability of Li-S battery with high-loading S cathodes and lean amount of electrolyte, and durable electrolyte and additives for long-term cell cycling and instability of the Li-metal anode. All these proposed future research challenges or barriers are key to realize the practical application high energy Li-S batteries. In conclusion, the reviewer thought the PI has proposed an excellent future research.

Reviewer 2:

The reviewer noted that this is the final year of this project and that the project team will accomplish the remaining milestones for FY 2019.

Reviewer 3:

The reviewer wrote that milestones indicate this project will demonstrate a high Li-conductive S cathode enabled by sulfide solid electrolyte. The reviewer added that more work is needed in the cathode composite with solid electrolytes. Also, the calculation of S content in the cathode composite should include the weight of electrolyte (liquid or solid).

Reviewer 4:

Regarding the scale-up preparation of the S cathode, the reviewer inquired about what would be the level. The reviewer also said the new design of cathode architecture is a practical target, from already accomplished specification (E-S equal to 4) to the target specification (E-S less than 3). The reviewer asked what the target cycle life is.

Reviewer 5:

The reviewer found that significant challenges still remain to get a durable Li-S cell with a dense S cathode and lean amount of electrolyte, i.e., low S utilization rate of a high-loading and low-porosity S electrode. To this end, the preparation of a dense S cathode will be scaled up, a new design of cathode architecture that will enable better utilization of S with lean electrolyte will be developed, and in situ and ex situ studies will be made to understand the S reaction pathway and degradation processes. Finally, the reviewer added, comprehensive approaches of new electrolyte and additives, separator coating, and Li protection will be adopted to extend the cycle life of Li-S cells.

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

Reviewer 1:

The reviewer stated that a ow-cost Li-S battery with longer cycle life is a potential direction to make a low-cost, large-capacity battery for electric vehicles.

Reviewer 2:

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

Reviewer 3:

The reviewer replied that this project is on Li-S rechargeable batteries. This battery chemistry can be both low cost and high energy. The reviewer explained that this project addresses the most challenging issues within Li-S chemistry, including limited cycle life, low S loading and low S utilization, and the S shuttle effect. The project also made a meaningful discovery and measurement of Li-S cycle life to electrolyte E-S ratio, and S- Li metal ratio. These numbers are important to understand the Li-S practical energy density.

Reviewer 4:

The reviewer indicated that Li-S batteries represent one of most promising next-generation high-energy-density storage systems, due to the very high theoretical capacity (1650 mAh/g) and high enrichment on earth. However, to realize the practical application of high energy Li-S batteries, many key barriers need to be solved, like the shuttle effects of polysulfides, unstable interface between the electrolyte and Li-metal anode, realizing the stable cycling of the S cathode at high loading and low E-S ratio, etc. The reviewer found that the PI has focused directly on these key barriers and proposed corresponding effective approaches. So, the reviewer thought this project supports the overall DOE objectives.

Reviewer 5:

The reviewer noted that Li-S can potentially offer 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 agreed that the resources are appropriate for the scope of the project.

Reviewer 2:

The reviewer found that resources are sufficient for the project to achieve the stated milestones in a timely fashion.

Reviewer 3:

The reviewer remarked that with 3 months left for conclude the project, the project team needs to achieve the target milestone of E-S less than 3 in a timely fashion. Based on what the project team has already accomplished, the reviewer thought they should have sufficient resources to reach the target specifications.

Reviewer 4:

The reviewer said resources are appropriate.

Reviewer 5:

The reviewer indicated resources for the current project to achieve the stated milestones are sufficient.

Presentation Number: bat286
Presentation Title: Lithium-Air Batteries
Principal Investigator: Khalil Amine (Argonne National Laboratory)

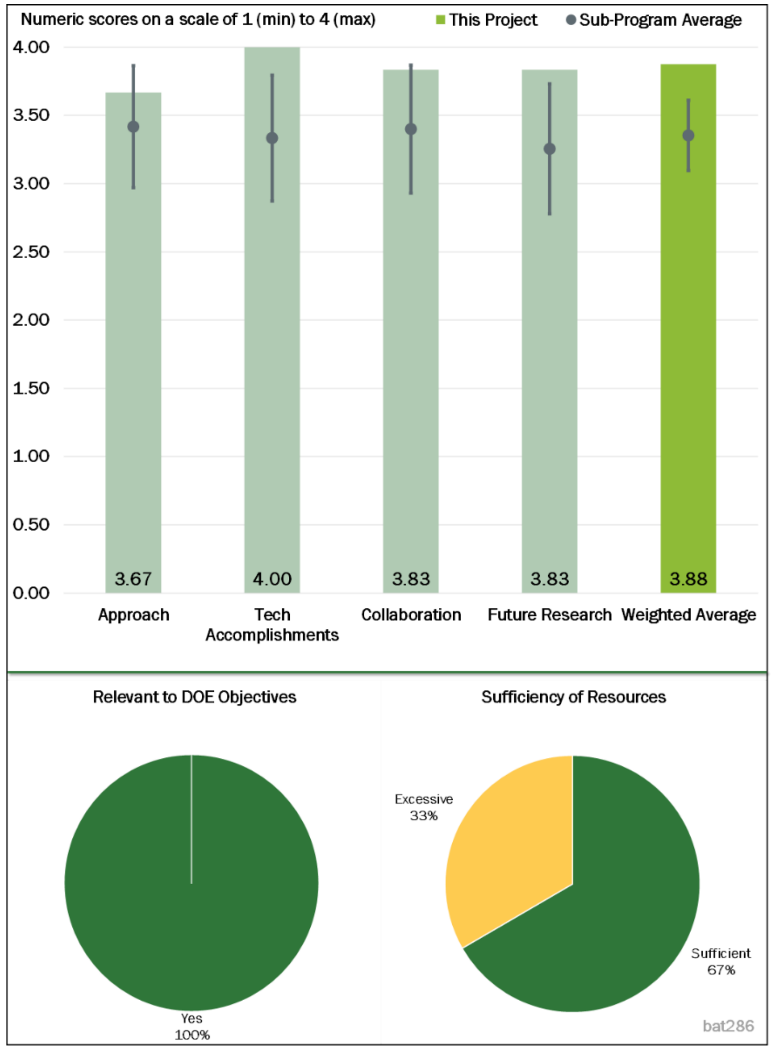

Figure 2-25 – Presentation Number: bat286 Presentation Title: Lithium-Air Batteries Principal Investigator: Khalil Amine (Argonne National Laboratory)

Presenter

Khalil Amine, Argonne National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

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

Reviewer 1:

The reviewer found that the team combined experimental and theoretical approaches to improve the performance of a lithium superoxide (LiO_2) battery, adding that this strategy has been adopted by many researchers and seems to work fine in this project.

Reviewer 2:

The reviewer commented that the PI and associates aim to address the low efficiency of a Li-air battery, which is one of the key barriers to the system. Both numerical modeling was used to understand the fundamental aspect of catalytic redox reaction of oxygen, while electrochemical methods including AC impedance was used to evaluate the effectiveness of the Co_2Ni catalyst developed in the project. The reviewer found that the approaches are adequate.

Reviewer 3:

This reviewer explained that the research activity focuses on development of the air electrode for a Li-air rechargeable battery. The team is developing an effective non-noble metal catalyst (i.e., Co and Ni particles embedded in LiOH as a catalyst [Co_2Ni@LiOH]) to decrease the over-potential and improve the air-cathode cycle life. The reviewer elaborated that the Li-air battery has many challenges, although it promises very high energy density. An air cathode is a particularly challenging area to improve, considering the complexity of the system and the stability of LiO_2 products. The catalyst facilitates the breakdown of Li_2O in the air electrode and is needed in order to reach a reasonable round-trip energy efficiency. To this end, the reviewer concluded that this work addresses part of the most important issues in a Li-air rechargeable battery.

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 indicated that the most unique accomplishment of the project is the Co_2Ni@LiOH electrode, which provides lower charge potential and thus better round-trip efficiency. The experiment testing and DFT calculations help understanding the mechanism.

Reviewer 2:

The reviewer indicated that team has made significant progress in the review period to include developing a non-noble metal Co_2Ni/LiOH catalyst; using morphology control to the catalyst to increase its efficacy; integrating into cells to verify performance; and performing molecular dynamic simulation to understand the improvements. The reviewer added that this catalyst decreases the charge potential by 0.5-3.5V compared to the one without the catalyst.

Reviewer 3:

The reviewer said that great progress has been made in the past year, explaining that a CoNi catalyst was synthesized. Significantly reduction of the oxidation potential during charging a Li-air cell was demonstrated. The enhancement of electrode conductivity was also illustrated. A low donor number electrolyte was identified for the improvement of the cycle life. One suggestion the reviewer made is that the full discharge instead of partial discharge should be used for evaluation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

This is a collaborative project with scientists in both the experimental field and the simulation field. The project team also collaborates extensively with scientists from other institutions, including university and National Laboratories.

Reviewer 2:

The reviewer found the collaboration among National Laboratories and universities is well coordinated, adding that there is synergy among the expertise of collaborators for the project objectives. The reviewer recommended that an industry member should be included in the collaboration. Even though Li-air is at very early stage, an industry member can provide some guidance on feasibility.

Reviewer 3:

The reviewer noted that collaboration team includes a National Laboratory and universities. For such a project with great application potentials, the reviewer recommended to get an industrial company 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 explained that the team proposes to work on other areas of Li-air batteries in the future. These include electrolytes additives, new oxygen electrode designs, and Li-metal electrodes. These are all important areas for a Li-air battery.

Reviewer 2:

The reviewer wrote that proposed future work is based on the current success and that the PI proposed to do a comprehensive study on electrolytes and further optimize the ai- cathode structure. Both are in line with the overall objective and the project goals.

Reviewer 3:
The reviewer said the proposed future work is still all basic research, which is understandable. The emphases are on the electrolytes and anode protection, as well as lowering the cost of the catalysts. The reviewer thought the proposal is kind of too general.

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

Reviewer 1:
The reviewer responded that the project strongly supports the DOE new energy competitive objective. Electrochemical energy storage has a broad impact on the U.S. energy landscape and the U.S. economy and is a very important program for DOE. The reviewer elaborated that a Li-air rechargeable battery has very high theoretical energy density, and it has the most challenges among all the battery systems. This is a long-term research topic. The reviewer concluded it makes sense for DOE to support this kind of long-term research effort.

Reviewer 2:
The reviewer wrote that the LiO_2 battery has great potentials for applications in electric vehicles.

Reviewer 3:
The reviewer remarked that Li-air chemistry is one of a couple of candidates for the beyond Li-ion system. There are obstacles that need to be addressed, namely, efficiency, cycle life etc. The proposed research aims to develop a new catalyst and electrolyte system, so the redox reaction of oxygen can become more reversible and can cycle for longer time.

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 project seems to be going well, with all milestones completed or on track. The project team has strong expertise in materials synthesis, characterization, and theory.

Reviewer 2:
The reviewer stated that ANL is very well equipped to carry out the proposed research.

Reviewer 3:
The reviewer indicated the resources are sufficient.

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

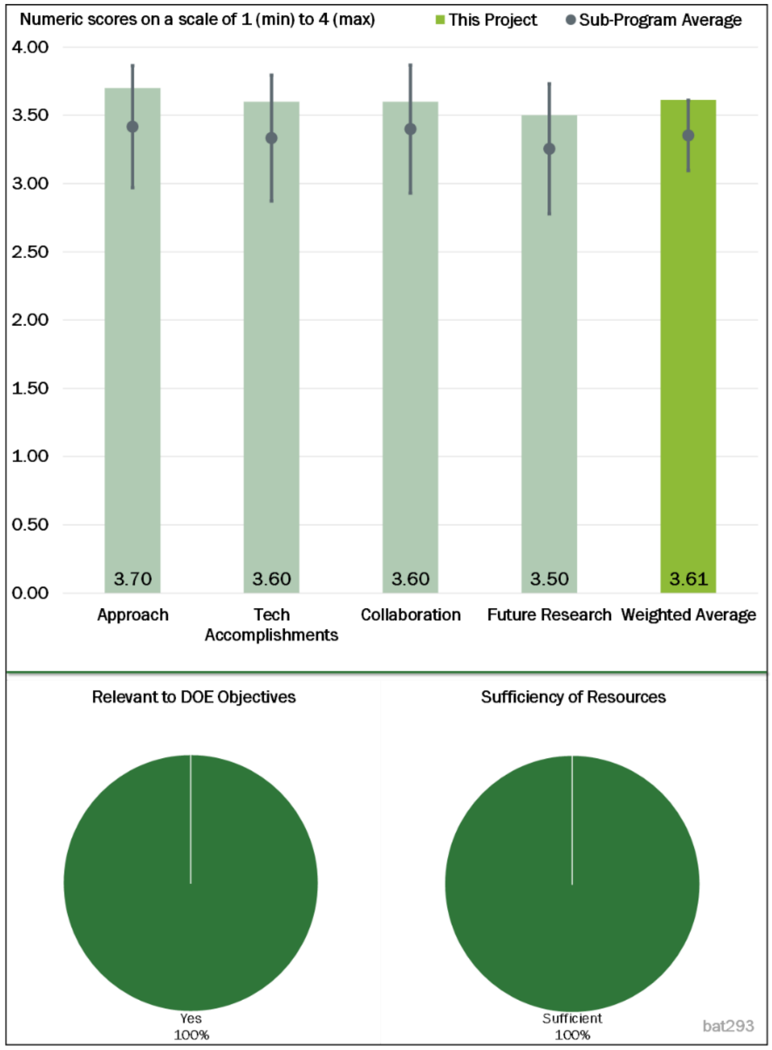

Figure 2-26 – Presentation Number: bat293 Presentation Title: A Closed-Loop Process for End-of-Life Electric Vehicle Lithium-Ion Batteries Principal Investigator: Yan Wang (Worcester Polytechnic Institute)

Presenter

Yan Wang, Worcester Polytechnic Institute

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 concluded that this group appears highly focused on the critical barriers for recycling. They are well integrated with commercial partners like A123, who are critical for providing guidance to ensure the relevance of what the Worchester Polytechnic Institute (WPI) team is doing. The reviewer added they are clearly organized and focused on the goals.

Reviewer 2:

The reviewer responded that the results indicate a better performance than the baseline material, which is an outstanding result. The project is well designed with good collaborations with the right groups. The fact that the investigators can work at scale to produce kilogram levels of cathode materials is quite impressive for an academic institution.

Reviewer 3:

The reviewer replied that the approach is very reasonable.

Reviewer 4:

The reviewer stated that the project is directly focused on materials supply and indirectly on sustainability of battery materials. The performance of the batteries produced from recycled materials is also addressed. The still-open question is if the secondary raw materials will be less expensive than the primary. The economic aspects are not presented by the project team yet.

Reviewer 5:

The reviewer explained that the approach is an extension of the approach used during Phase 1 with NMC-111 recycled material. The data being generated with this approach can be used in general to make reasonable evaluations of the recycling process in terms of performance. However, it was not clear to the reviewer from the work presented how much variability in feedstock can be successfully handled with this specific recycling process. While the results are impressive so far on NMC-622 materials (similar to the earlier results on NMC-111), the approach would be better if it clearly included a wide range of feedstock materials in terms of chemistry, binders, anodes, previous history, etc. The reviewer suggested that the approach should include enough variability in feedstock to be able to figure out the processing window—that is, how far from "typical material" can one go before the recycling process fails to produce satisfactory 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 found that the project is clearly making excellent progress. For the set of materials being tested in the recycle process, the project team is on schedule and producing valuable data on the viability of the process. The reviewer concluded that there is a high likelihood that the rest of the Phase 2 milestones will be met on schedule.

Reviewer 2:

The reviewer wrote that the team appears to have excellent results on producing cathode materials from spent Li-ion batteries. Of course, the transition metals in the battery are only a small portion of the waste stream (there are also solvents, graphite, etc.), so this is not a complete recycling solution, but it is creating a way to recycle at least some of the contents. It sounds like the team is also thinking about where the other waste streams may go. Overall, the reviewer deemed there to be excellent progress and a good publication in scientific reports.

Reviewer 3:

The reviewer remarked that the investigators are on track and are meeting the milestones, adding that impressive results have been obtained in terms of scalability and performance.

Reviewer 4:

The reviewer said it appears to be making solid progress as well as developing a business operation.

Reviewer 5:

The reviewer wrote that while technical accomplishments look in overall good, there is still a lot of room for improvement. The reviewer provided the following comments and suggestions: First, the details of the recycling process are not given; second, it would be desirable to understand the reason why the recycled NMC-111 shows better cycle-life performance compared to the commercial powder; third, a full understanding of why 11 Ah cell-cycle life is inferior to 1 Ah cell in Phase 1 and improving the 11 Ah cell would be required; and fourth, a comparison of the 11 Ah Phase 1 cells from three different lots shows well grouped, better performances of the tested cells, distant from the commercial, 26-Ah reference cell. However, the parameters of the reference cell (e.g., active material loading per square centimeter and optimization more toward the energy, not the power) may be not equivalent to the tested cells. In such a case, a natural would be to observe worse-rate performance of the reference cell. In the opinion of the reviewer, there should be executed rate-performance test on the cell of the same capacity, materials loading etc., prepared by the project team from the commercial material, following the production process that was applied to the cells made of recycled materials.

The reviewer continued that, fifth, NMC-622 coating nor coating process are not presented nor were SEM images explained; sixth, a comparison of Phase 2 single-layer pouch cells shows huge differences between different cells from the same lot, including the control cells. This indicates large variability of the method used, which makes the result of low credibility. The project is advised to improve the method or an alternative one, giving more precise information. Lastly, the future cells chemistry may be not compatible with the developed technology. There might be technical and economic issues encountered. Some action to avoid or minimize the influence of such issues would be required.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer wrote that integration with A123 is crucial for this effort, to truly assess the cathode powders produced, and it appears the team is doing so well.

Reviewer 2:
The reviewer said the list of collaborators looks very good.

Reviewer 3:
The reviewer commented that the WPI team is clearly working well with their A123 collaborators, which is apparent from the pace of activities—from obtaining material for recycling, to the recycling process itself, to new cell fabrication, and finally electrochemical performance determinations. The reviewer remarked that the role of ANL in testing to date could have been clearer in the presentation—most of the testing appears to have been done at A123 where the cells were made. If ANL has participated in some or all of the Phase 2 testing, the reviewer suggested that that should be made clearer in the presentation of the results. Otherwise, the collaborations seem to be working fine to this point.

Reviewer 4:
The reviewer found the collaboration between the business and university appears to work.

Reviewer 5:
The reviewer stated that it appears that good collaboration exists between A123, WPI, and battery resources, but added that for other collaborators, it appears less easy to judge the level 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 found the program is well planned from a program management viewpoint. Because this is follow up from a Phase 1 project, the reviewer added, the path forward is clear and laid out in a logical manner.

Reviewer 2:
The reviewer said the team is focused on scale-up and continued integration with A123, both good strategies for future work.

Reviewer 3:
The reviewer wrote that project is complete and added that clearly a full business proposal and operation are next. The reviewer noted that such a plan would have too many sensitive details to publicly disclose the future.

Reviewer 4:
Similar to the comment referenced about the approach, the reviewer asserted that future work could be improved by specifically including materials with a wide enough variability in quality to be able to determine the limits of the recycling process—that is, at the point where the process fails to produce satisfactory recycled material. But, in general, the future research plan is reasonable and should answer basic questions about the viability of the recycling process developed at WPI.

Reviewer 5:
The reviewer indicated the proposed future research is covering the remaining barriers and challenges; however, the future new chemistries and their influence on the technology should be better addressed.

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

Reviewer 1:

The reviewer remarked absolutely, noting that vehicles must be recycled. The reviewer elaborated that 10 million new vehicles per year means almost that many retired every year. Additionally, batteries are unique and contain precious metals and toxic chemicals. The reviewer liked that more than NMC was recovered. The reviewer praised as a good job that the DOE is addressing this issue.

Reviewer 2:

The reviewer found that the objectives of the program clearly address DOE objectives to support the development of a battery recycling industry for commercial Li-ion cells, adding that the alignment with DOE's initiatives in recycling is very good.

Reviewer 3:

The reviewer said the project is clearly contributing to DOE goals.

Reviewer 4:

The reviewer wrote that battery recycling is of high importance for battery sustainability and for securing the raw materials availability, and thus supports the DOE objectives.

Reviewer 5:

The reviewer indicated that this program supports reducing the cost of Li-ion batteries because the recycled material is of lower cost than baseline per the discussions with the PI. It also addresses the issue of shortages of critical battery materials such a Co, Ni, and Li.

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 project advancement indicates the sufficiency of the engaged resources.

Reviewer 2:

The reviewer found that the resources are sufficient (but certainly not excessive) to complete the work described in the remainder of Phase 2. The reviewer had no concerns, adding that the PI seems to have been able to manage the resources efficiently to date.

Reviewer 3:

The reviewer indicated the budget seems to be sufficient to demonstrate the viability of this recycling technology. Hopefully, the reviewer said, it will attract future funds from the private sector.

Reviewer 4:

The reviewer replied that resources appear appropriate.

Reviewer 5:

The reviewer cannot judge: It looks like the project team did the job with what it had.

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)

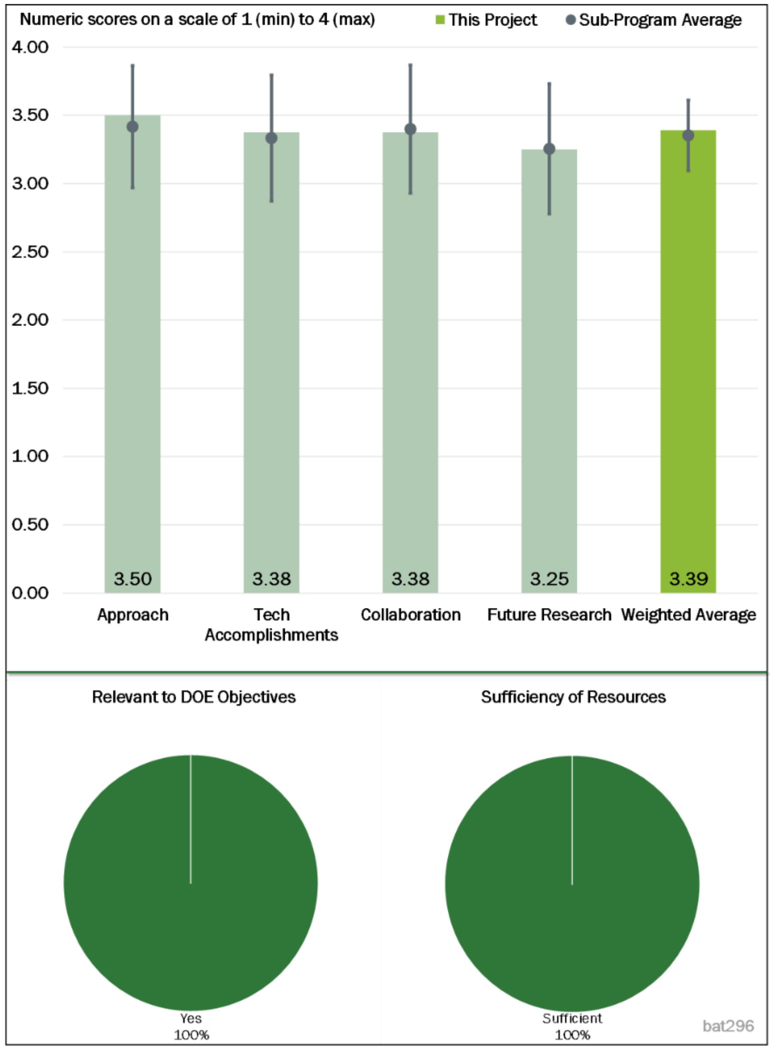

Figure 2-27 – Presentation Number: bat296 Presentation Title: Development and Validation of a Simulation Tool to Predict the Combined Structural, Electrical, Electrochemical, and Thermal Responses of Automotive Batteries Principal Investigator: Chulheung Bae (Ford)

Presenter
Chulheung Bae, Ford

Reviewer Sample Size
A total of 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 the project approach was well reasoned and structured. The reviewer elaborated that the plan addresses the objective of developing a simulation tool to predict the influences of abuse on a battery cell and module to reduce the design, build, and prototyping cycle time. Dividing the activities into experimental validation, solver validation, and the development of new models makes the objectives of each piece clear and pursuable.

Reviewer 2:
The reviewer affirmed that the PI's team has successfully developed a simulation tool to predict the combined structural, electrical, electrochemical, and thermal (EET) responses of automotive batteries to crash-induced crush and short circuit, overcharge, and thermal ramp and validate the tool for conditions relevant to an automotive crash. The reviewer concluded that the project is well designed and feasible to realize the targets in terms of the cost reduction and abuse tolerance

Reviewer 3:
The reviewer wrote that model development and validation combine together to solve the challenges on cost and abuse tolerance.

Reviewer 4:
The reviewer stated that the approach designed to accomplish the target is reasonable.

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 indicated that project progress was planned and accomplished well.

Reviewer 2:
The reviewer noted that X-ray tomography, development of models with layered solid elements under different abuse, and initiating the development of the macro model are all accomplishments that are part of the overall goals of this project.

Reviewer 3:
The reviewer explained that PI's team has developed a predictive simulation tool to shorten or eliminate design, build, and test prototype cycles and to accelerate development and optimization of crash protection systems robust enough to meet safety requirements. The calculation was conducted in a pouch cell model containing 2 pouch layers at the top and bottom, 17 total cell layers, 556 elements per layer, and 76,728 solid elements.

Reviewer 4:
The reviewer remarked that the project is in its 4th year and as a result, one would expect more progress to have been made with validation of the simulation-tool set. It was clear to the reviewer that delays with equipment from the previous test supplier have prevented this portion of the work, yet validation is crucial and should have been prioritized within the first 2 years. Significant progress has been made to reduce the computational resources needed for this tool by simplifying the model with layered solid elements. This is valuable for application and has been demonstrated for the mechanical and thermal solvers. It is unclear, however, without experimental data if creating two models that behave the same or differently are (either one) representative of a real system. There also need to be further discussion of how the material models take into account the granular nature of the electrodes. The reviewer wrote that no mention is made of how different formulations and processing conditions could affect the simulation results.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said there is wide project collaboration with several National Laboratories, academia, and industrial companies.

Reviewer 2:
The reviewer noted that ORNL developed methods to scale up detailed mechanical simulations to reduce computational complexity while retaining high fidelity. The reviewer explained that LS-DYNA® is the computer-aided engineering (CAE) software of choice for the project and contains key, battery-specific solver enhancements. The reviewer added that the Southwest Research Institute has designed the prototype tests stands and is running model validation tests.

Reviewer 3:
The reviewer stated that the roles of each collaborator are clear.

Reviewer 4:
The reviewer wrote that collaboration across the team is adequate.

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

Reviewer 1:
The reviewer indicated that the proposed future research is reasonable and feasible based on current progress. One suggestion from the reviewer is that the high-speed impact experiment needs to be performed as soon as possible.

Reviewer 2:
The reviewer offered that the future research topics look great. The reviewer suggested, however, to add the test at different SOC and state of health (SOH) to valid the model.

Reviewer 3:
The reviewer referenced the presentation: "Additional crush tests are designed and will be carried out with 0% SOC cells for non-destructive analysis of the deformed cells…." The reviewer asked if different levels of SOC will influence the simulation results.

Reviewer 4:
The reviewer remarked that the proposed future work is quite significant with the amount of time remaining. The modeling strategy should have been simplified earlier in the project in order to use this later time for validation and expansion of the model to module level simulation. The reviewer found that there is significant risk that this project may require additional time to complete in order to generate a usable tool set.

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

Reviewer 1:
The reviewer agreed that this project well supports the DOE objectives. To predict the response of deformed batteries after a short circuit occurs is highly needed. To predict the combined structural and EET responses of automotive batteries to crash-induced crush is very important.

Reviewer 2:
Noting that safety is one of the most critical parameters for Li-ion batteries, the reviewer wrote that this project aims to understand the safety mechanism of Li batteries under abuse condition (mechanical impact), so that research can design safer Li batteries.

Reviewer 3:
The reviewer replied that abuse tolerance of batteries is important for safety considerations of batteries for electric vehicles.

Reviewer 4:
The reviewer wrote that this project addresses the need to better understand abuse tolerance in large-scale cells and packs. However, the reviewer commented, while the simulation tool set would foreseeably reduce the development cost of battery design by reducing validation time, the results in their current state are not useable for this end. The reviewer concluded that much additional work would be necessary to generalize and align the simulation models with real systems of varying format, production methods, materials, abuse conditions, etc.

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

Reviewer 1:
The reviewer wrote that the resources are enough for the proposed research.

Reviewer 2:

The reviewer said the resources for this project are sufficient, but that more time will likely be needed for completion.

Reviewer 3:

The reviewer observed that some tasks are a bit behind schedule.

Reviewer 4:

The reviewer stated that high-speed impact testing has not been performed due to lack of sophisticated equipment and resources at the previous test supplier company and that extensive analysis of the deformed cells is still required to better define the failure mechanisms.

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

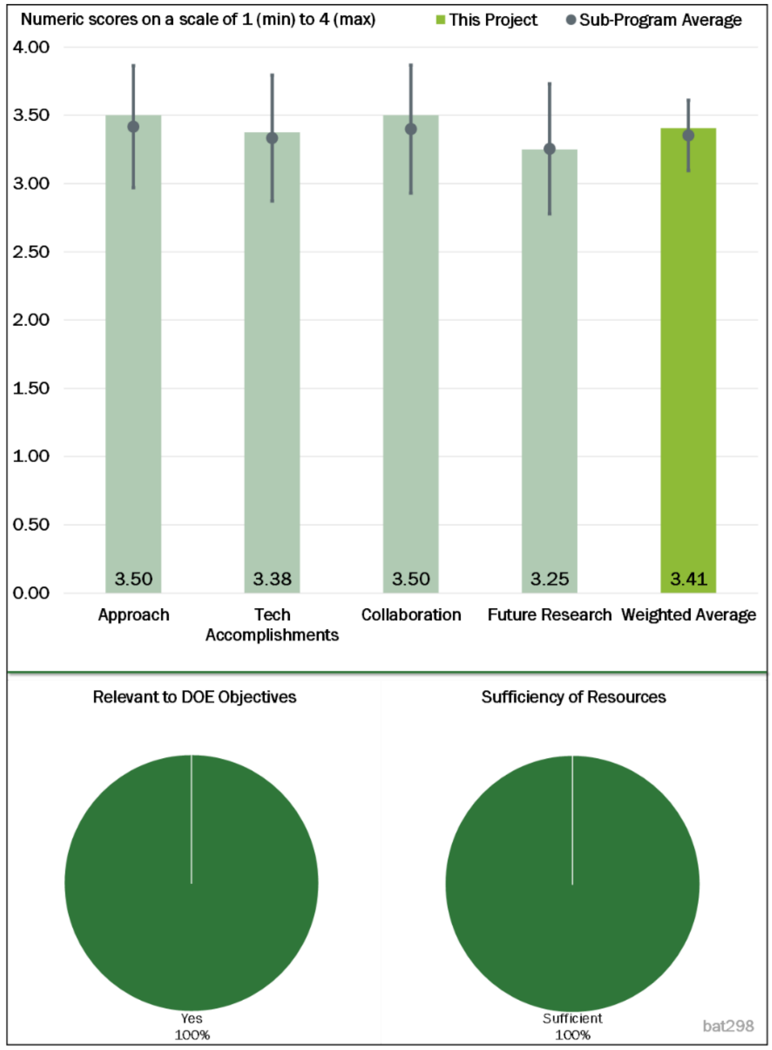

Figure 2-28 – Presentation Number: bat298 Presentation Title: Efficient Simulation of Mechanical-Electrochemical-Thermal Abuse Phenomena in Lithium-Ion Batteries Principal Investigator: Shriram Santhanagopalan (National Renewable National Laboratory)

Presenter

Shriram Santhanagopalan, National Renewable 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 explained that the objectives of this project are to develop effective simulation tools to integrating the mechanical failure and abuse of Li-ion batteries and to assess the safety of Li-ion batteries more efficiently. The project team has proposed a multiscale, simultaneous coupling and constitutive model to develop the simulation tools. The results show the developed model can simulate that the single-cell repose on the three-dimensional (3-D) prismatic geometry takes approximately 23 minutes. The project team also proposed mechanical modeling to finish the abuse response of Li-ion batteries under mechanical strain. The results show that the simulation tools can perform the simulation. Therefore, the reviewer thought the approach to performing the work proposed by the PI's team is feasible and excellent.

Reviewer 2:

The reviewer concluded that the approach of mechanical-electrochemical-thermal model development is a good tool to evaluate abuse response of batteries for practical assessment of battery safety.

Reviewer 3:

The reviewer said the approach designed to accomplish the target is reasonable.

Reviewer 4:

The reviewer found that the project approach is generally effective toward the goal of creating modeling tools to better understand and simulate abuse conditions in Li-ion batteries. However, the breadth of the project and the large number of partners (including four National Laboratories) makes it appear unfocused in its goal of creating specific tools with defined outputs. As a result, the reviewer concluded, there is no clear outcome that is practically useable by industry partners and little in the way of examples (via experiment) to further our understanding of the battery design-abuse relationship.

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's team has achieved all the milestone very well, as demonstrated by the proposed modeling and simulation results. The reviewer added that modeling tools can simulate and integrate the mechanical failure and abuse response of Li-ion batteries. So, the reviewer concluded, the technical accomplishments and progress as evaluated are excellent.

Reviewer 2:

Quoting from the presentation: "…models developed by NREL under [computer-aided engineering for batteries] CAEBAT] have been licensed out to 7 different entities." The reviewer remarked that this is impressive.

Reviewer 3:

The reviewer said the project progress was well planned and well accomplished.

Reviewer 4:

The reviewer remarked that the project is in its 4th year, yet it is unclear what the final united output of this work will be. Progress has been made to improve computational efficiency of the modeling tools and enable user-defined elements in the scheme. Experimental data have been added addressing strain, temperature, and aging on mechanical responses to abuse. These data are quite valuable but do not appear correlated (so far) with the modeling portion of the work. The reviewer noted that one claim of the work is to expand predictive simulation to the module level, but no information about this effort is given. For use by industry partners, module-level simulation should be prioritized.

The reviewer noted that cell-level case studies have been defined in the past year, but no test results have been shown. After 4 years, experimental validation should have been a greater priority. The defining of these case studies is not particularly relevant to automotive applications and the limited number of cell formats is a significant oversight in this respect. Variations in interior cell and electrode (formulation and processing) design should be similarly prioritized in case studies. The reviewer concluded that the outputs of this project would be more significant if it were focused on specific research questions or well-defined systems rather than the creation of tools and databases.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

According to the reviewer, all the partners have participated in the project very closely and are well coordinated. All the partners utilize their advantages to solve many problems in each part of the project. Based on the accomplishments and progress of this project, the reviewer thought the project team has an outstanding collaboration and coordination across the project.

Reviewer 2:

The reviewer said there is wide project collaboration with several National Laboratories, academia, and industrial companies.

Reviewer 3:

The reviewer wrote that collaborators include National Laboratories, universities, and industry.

Reviewer 4:
The reviewer found that collaboration across the project teams is unclear given the number of partners and the proportionately small amount of funding for each.

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 is based on the progress of this project. Many improvements, like validation of the simulation on more cases, building the database, etc., are reasonable and necessary to be further studied. So, the proposed future research plan deserves to be supported and also is excellent.

Reviewer 2:
The reviewer suggested also studying the aged battery module (especially the aged module component).

Reviewer 3:
The reviewer asked whether the model for a multi-cell validation case study can be expanded to battery pack level.

Reviewer 4:
The reviewer commented that the proposed future work does not appear focused toward a specific goal. There is questionable value to a project that "expands the user base" and creates databanks of information without knowing if the intended users need or see significant use for these tools.

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

Reviewer 1:
The reviewer wrote that safety is one of the critical factors for batteries, which is highly related to the DOE objective.

Reviewer 2:
The reviewer replied that developing safe Li-ion batteries and developing suitable simulation tools to simulate the safety of Li-ion batteries are important for practical application. So, as a result, the project definitely supports the overall DOE objectives.

Reviewer 3:
The reviewer affirmed that model development for assessment of battery safety is important for battery applications in electrical vehicles.

Reviewer 4:
The reviewer found that this project addresses the need to better understand abuse tolerance in large-scale cells and packs. However, the reviewer added, while the tools developed in this project could be of use to industry partners, they are largely unvalidated. It is unknown how much these tools will reduce the development cost of new battery cells, modules, and packs.

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 resources for this project are sufficient.

Reviewer 2:

The reviewer found that the resources for the current project are sufficient to achieve the stated milestones.

Reviewer 3:

The reviewer said milestones are completed on track.

Reviewer 4:

The reviewer wrote that the resources are enough for the proposed research.

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

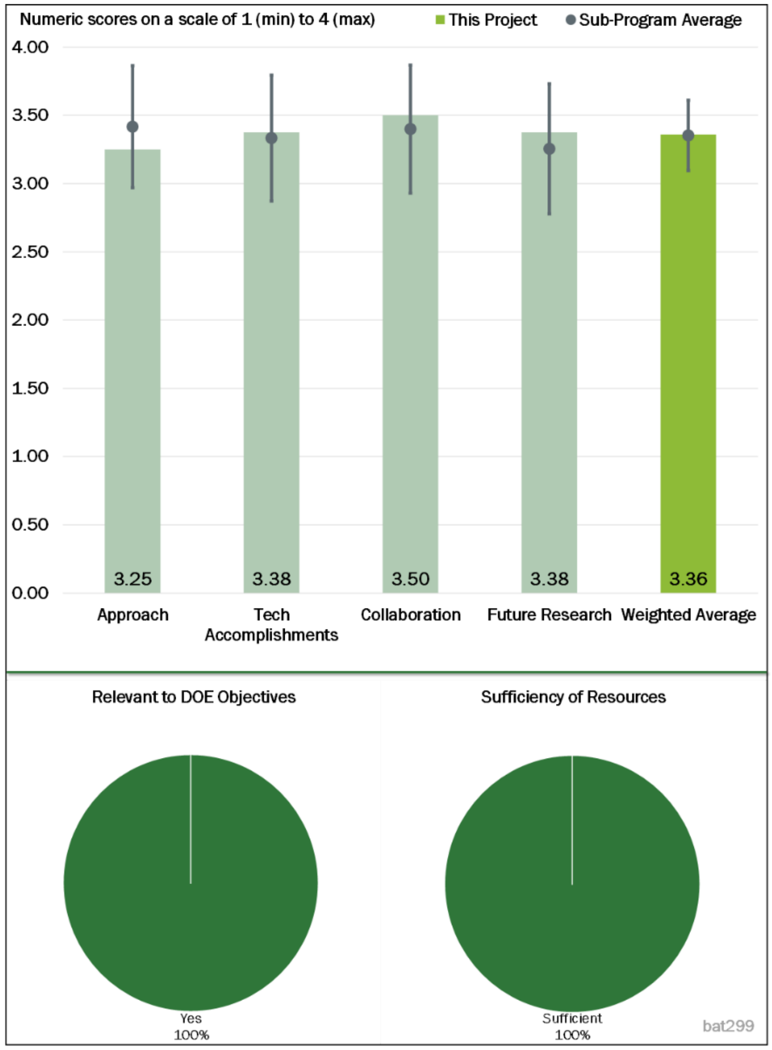

Figure 2-29 – Presentation Number: bat299 Presentation Title: Microstructure Characterization and Modeling for Improved Electrode Design Principal Investigator: Kandler Smith (National Renewable Laboratory)

Presenter

Kandler Smith, National Renewable 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 wrote that microstructure analysis and 3-D microstructure modeling will bridge the gap between modeling tools and the cell-design process in industry.

Reviewer 2:

The reviewer said that the approach designed to accomplish the target is reasonable.

Reviewer 3:

The reviewer commented that the approach to the technical work is appropriate given the goal of this project to create tools for microstructure modeling of battery components. Such tools have been created and made user-friendly, numerical simulation has been improved, and models have been extended to new relevant problems (i.e., Si anodes). However, the reviewer wrote, it was challenging to see how industrial partners may use these tools with so little experimental validation of the outcomes.

Reviewer 4:

The reviewer remarked that Li plating leads to severe capacity fading and possible safety problems in Li-ion batteries. Thus, non-destructive detection methods for Li plating are critical for safe and reliable operation of Li-ion batteries. The project is well designed and feasible. The different polarization of the electrode with different thickness should be considered in the simulation models. The reviewer concluded that simulation models need to be checked with more experiments under different extreme 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 noted that the team improved robustness and speed of the 3D microstructure high-performance computing model and reformulated the classical Pseudo2D electrochemical model to efficiently incorporate large deformation at particle and electrode levels. Taking advantage of the electrode capacity and cell-voltage sensitivity with the tortuosity factor, the macro-homogeneous model has helped to validate the microstructure-predicted tortuosity factors, showing fitted values in good agreement.

Reviewer 2:

The reviewer referenced the presentation: "microstructure analysis tool is developed and will be published open-source." The reviewer remarked the developed model is an extension to other battery systems (Si, Li_2S and polycrystalline).

Reviewer 3:

The reviewer said the project progress was planned and accomplished well.

Reviewer 4:

The reviewer found that the outcomes of the project, beyond the creation of a tool set, are quite interesting (i.e., the analysis of open-circuit potential [OCP] with Si that is stress dependent). The reviewer added that the improvement of calculation time is an achievement but does not have relevance unless the model is used broadly. The creation of idealized microstructures and the analysis of electrochemical and mechanical properties are valuable, but unfortunately, there is no reported validation of the schemes being studied.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Noting that five institutions are working on the project, the reviewer indicated that the roles are assigned to them respectively to include: electrode and cell prototyping and characterization, stochastic electrode reconstruction and carbon-binder domain generation for microstructure studies, nano- and micro- X-ray computed tomography, tortuosity measurement, NMC-811 samples with different size distribution, and mud-cracking. The reviewer concluded the collaboration and coordination are very good.

Reviewer 2:

The reviewer agreed the roles of each collaborator are clear.

Reviewer 3:

The reviewer said the project features wide collaboration with several National Laboratories and universities.

Reviewer 4:

The reviewer concluded that collaboration across the project team appears adequate as this is a part of a larger 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 indicated that the proposed future work should be quite interesting, adding that enhancements by including carbon and binder will be key. Adding in effects from various crystal structures and particle-size distributions will also prove the value of the toolset. Though this is part of a larger project that involves experimental work, the reviewer suggested that more emphasis should be placed on validating the outcomes from this model. Likely more time will be needed to complete this work.

Reviewer 2:
In the future research, the reviewer wrote, more factors on batteries should be considered in modeling, and that the developed models need to be validated by more experiments (using different rate, temperature, electrodes material, electrolyte, and so on).

Reviewer 3:
The reviewer suggested applying models to design for higher capacity electrode materials (i.e., Si and S).

Reviewer 4:
The reviewer wrote that the project progress was well planned and well accomplished. But the reviewer suggested adding the electrode (cell) thickness change as the function of SOC and SOH.

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

Reviewer 1:
The reviewer agreed that this project supports the overall DOE objectives, elaborating that these results resolve the discrepancy in tortuosity-factor estimation that hindered the reliability and thus predictability of battery electrode macro-models, especially when used in thick electrodes and/or fast charge, which is critical for automotive application.

Reviewer 2:
The reviewer wrote that the models developed for mechanical failure of cells and packaging components are important for safe battery applications.

Reviewer 3:
The reviewer replied that the project proposed to develop validated modeling tools to accelerate development of batteries, in support of vehicle electrification R&D to reduce dependence on imported oil.

Reviewer 4:
The reviewer remarked that this project does address the need to better understand microstructure in electrodes, influences on electrochemistry, and abuse tolerance by using modeling. The reviewer further commented that there is no consideration of cost or energy density directly in this effort, although it could be addressed in other portions of the larger project.

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

Reviewer 1:
The reviewer stated that resources for the project are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 2:
The reviewer wrote that the tasks and milestones are completed.

Reviewer 3:
The reviewer said the resources are enough for the proposed research.

Reviewer 4:
The reviewer replied resources for this project are sufficient.

Presentation Number: bat300
Presentation Title: Consortium for Advanced Battery Simulation: Development of Computational Framework for Battery Analysis under Extreme Conditions
Principal Investigator: Srikanth Allu (Oak Ridge National Laboratory)

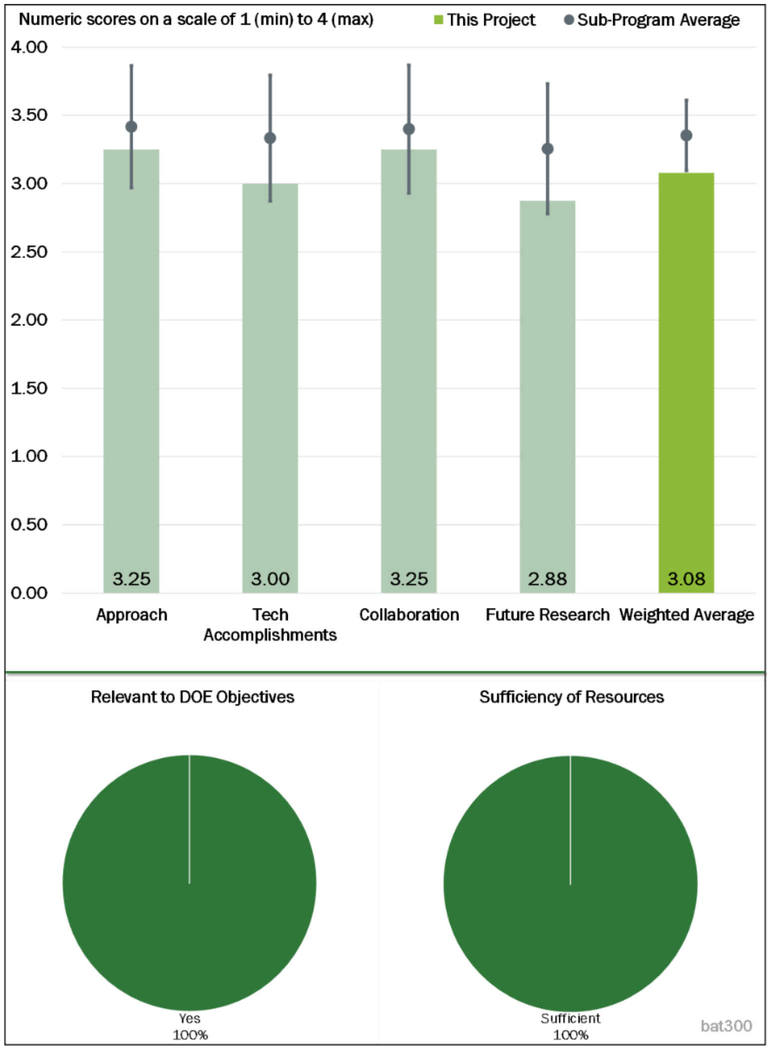

Figure 2-30 – Presentation Number: bat300 Presentation Title: Consortium for Advanced Battery Simulation: Development of Computational Framework for Battery Analysis under Extreme Conditions Principal Investigator: Srikanth Allu (Oak Ridge National Laboratory)

Presenter

Srikanth Allu, 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 wrote the clear view of cathode and Cu-current collectors can be obtained by non-destructive X-ray computed tomography (XCT) to identify failure mechanisms under compressive load. The reviewer agreed that the project is well designed. In the mechanical model, the reviewer suggested that the particle shape be considered, because the particle shape of the electrode materials may not be round actually. Moreover, the diameters of the electrode material particles are not the same as each other.

Reviewer 2:

The reviewer said the approach designed to accomplish the target is reasonable.

Reviewer 3:

The reviewer described the approach to the technical work as quite aggressive, namely attempting to use computation to assess the impact of electrode-component processing on cell performance and abuse tolerance. Given the many aspects being assessed (influence of particle size and shape, calendering, and electrode composition on modulus, Li^+ distribution, rate capability, plating etc.), it may be useful to focus on a single area of study (i.e., Li plating and Li^+ concentration or mechanical strength and abuse tolerance), especially given the limited time left in the project.

Reviewer 4:

The reviewer suggested using microstructure information for the mechanical model to understand failure mechanisms.

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 results from this project are both interesting and valuable. The experimental XCT results provide key findings regarding the mechanical strength of the Cu current collector. The ability to match full-cell electrochemical evaluation is impressive. The reviewer elaborated that flexibility of the model in particle size, shape, and electrode composition is fantastic. Also, findings on the relaxation of non-uniform Li^+ distributions during the CV portion of a CC/CV protocol is enlightening. The reviewer asked if this relaxation phenomena is time or bias dependent. The reviewer added that the one area that seems weak is in Li plating, as this is already deeply investigated by a number of other VTO-funded projects.

Reviewer 2:
The reviewer noted that a model for battery mechanics has been developed based on particle formation, microstructure characterization, and upscaling to a continuum model.

Reviewer 3:
The reviewer responded that the project team developed a framework for mechanics of battery-active materials based on particle assembly formation, non-local microstructural characterization, and upscaling to a continuum model. In validation of full-cell simulations of NMC-532/A12, the reviewer suggested adding more experiments (different rate cycling).

Reviewer 4:
The reviewer remarked that the project only accomplished 75% by the end of May, and it might be difficult to finish all planned items by September 2019.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found good collaboration and coordination across the project team.

Reviewer 2:
The reviewer said there is wide project collaboration with several National Laboratories, academia, and industrial companies.

Reviewer 3:
The reviewer said the collaboration across the project teams appears adequate.

Reviewer 4:
The reviewer said the team needs to specify the collaborators' roles.

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 proposed future work should be quite interesting, but there is not much time remaining in the project so likely not everything can be done. The reviewer suggested that further investigation of Li plating may not be valuable as this is being covered by the Xcel effort. The response to inhomogeneities in the electrodes is an important area of investigation as we have limited ability to find such areas experimentally. Additional XCT imaging could be valuable support.

Reviewer 2:

The reviewer asserted that more electrode materials should be tested to develop the computational framework for battery analysis. For example, thermal runaway features of different electrode materials are not the same completely. A computational framework developed from an electrode material cannot be applied in other electrodes materials. The reviewer added that the computational framework needs to be checked via different experiment conditions.

Reviewer 3:

The reviewer suggested the project team consider different electrode materials in the model development.

Reviewer 4:

There are several comments and questions from the reviewer, who asked what the Li-ion polymer, SST, is in the top right figure on Slide 5, and why this cell did not fail; and why the PI used XPS depth profiling on Slide 7. The reviewer noted that the overcharge result on Slide 8 is isolated from the main topic. Finally, the reviewer remarked that the research on the cycling performance test and Li plating is also isolated from the main topic.

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

Reviewer 1:

The reviewer remarked that these results are important for building safer batteries and providing information for the safety monitoring function of the battery-management system. So, the project supports the overall DOE objectives.

Reviewer 2:

The reviewer said that this project addresses the need to better understand microstructure and electrode-processing conditions in relation to impacts on cell performance. The focus on test cases and providing insight is important, rather than building tools for the sake of broad use.

Reviewer 3:

The reviewer indicated that the deformation and failure modes of Li-ion cells are important for battery applications.

Reviewer 4:

The reviewer stated that the topics are related to the DOE objective, but the reviewer felt they are isolated from each other.

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

Reviewer 1:

The reviewer wrote that tests in the project include micro- and nano-indentation to obtain strength and elastic properties of electrode secondary particles and micro-scratch tests to study aggregate strength. The compression and bending tests will be able to freeze the internal cell configuration and characterize its evolution. The reviewer concluded that resources are sufficient for the project to achieve the stated milestones in a timely fashion.

Reviewer 2:

The reviewer found that milestones have been completed as planned.

Reviewer 3:

The reviewer wrote that resources for the project are sufficient to achieve the target.

Reviewer 4:

The reviewer replied resources for this project are sufficient, although more time would be useful to complete additional work.

Presentation Number: bat309
Presentation Title: Electrode Materials Design and Failure Prediction
Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

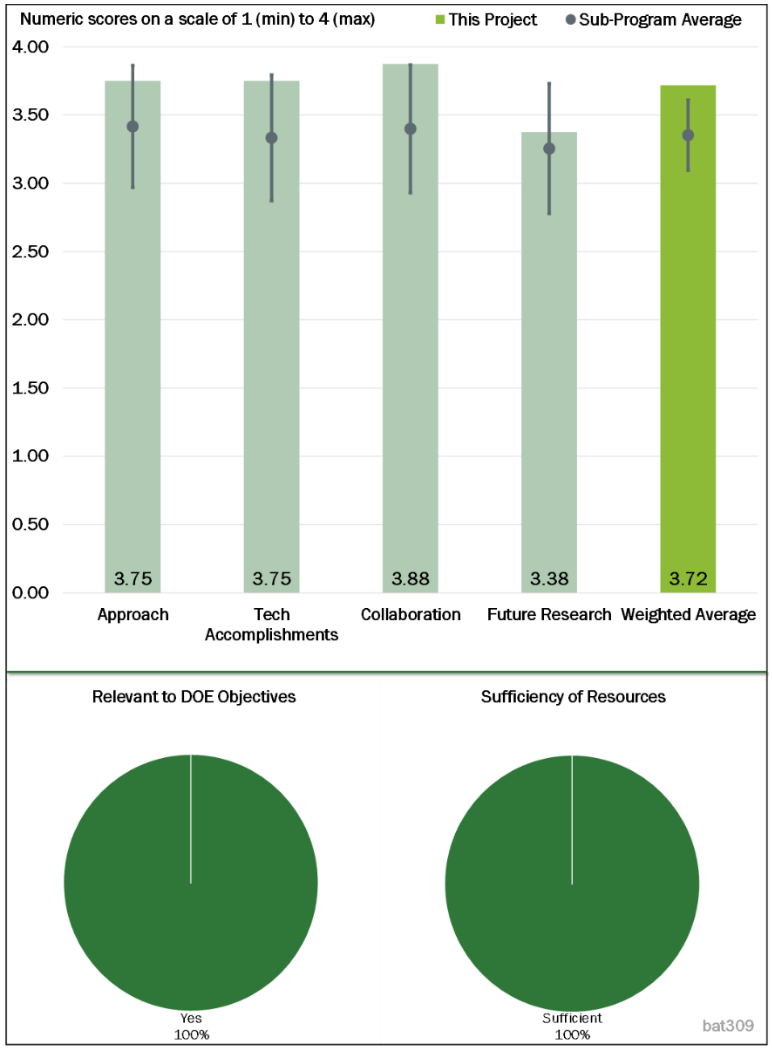

Figure 2-31 – Presentation Number: bat309 Presentation Title: Electrode Materials Design and Failure Prediction Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

Presenter

Venkat Srinivasan, 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 praised the very integrated approach to understanding the critical factors that lead to Li dendrites and poor cathode solid-electrolyte performance.

Reviewer 2:

The reviewer wrote that the technical barriers, such as the dendrite growth and performance decay due to interfacial delamination, are addressed well, and the progress made in the project clearly demonstrates its good design and feasibility.

Reviewer 3:

The reviewer said it was a good approach to gradually relax the Monroe-Newman assumptions. The reviewer suggested that future modeling consider a larger surface region than just one dendrite.

Reviewer 4:

The reviewer remarked that Li-dendrite growth and performance decay were addressed but more work is needed. The reviewer suggested use of an experimental design matrix with input and output variables and factor levels can help for future work to reach DOE goals more quickly.

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 results of Li-dendrite growth and cathode-SSE interface dynamics are excellent.

Reviewer 2:

The reviewer wrote that all technical accomplishments are relevant and stay in line with scheduled milestones. The project team was able to develop and apply their mathematical models to prediction of dendrite growth and delamination at the interface of the cathode and solid electrolyte.

Reviewer 3:

The reviewer stated that a number of experimentally testable predictions have been made, adding that the project team needs to wait until the experiments come in. The reviewer concluded that new insights are being provided.

Reviewer 4:

The reviewer replied that a mathematical model can predict dendrite growth and show delamination properties.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said the project team has a terrific group of people with different skills.

Reviewer 2:

The reviewer found very nice collaboration with experimental and theoretical groups, which supplement the PI's continuum-modeling expertise.

Reviewer 3:

The reviewer noted that the project team has been collaborating with DOE National Laboratories and academic universities and such collaboration seems very fruitful.

Reviewer 4:

The reviewer indicated the project seems to have worked fine between National Laboratories and with a graduate student from the University of Michigan.

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

Reviewer 1:

The reviewer described the future direction as clear and relevant, adding that incorporation of properties of actual SEI and cathode-electrolyte interphase (CEI) layers into the model will provide more insight into the dendrite-growth mechanisms and the overall failure prediction during the electrochemical cycling.

Reviewer 2:

The reviewer said the proposed future work appears to be spot on. The reviewer would encourage direct testing of model predictions regarding current homogeneity and Li-dendrite growth. The reviewer wondered if perhaps a model system incorporating an SSE with a defined defect could be tested.

Reviewer 3:

The reviewer indicated the proposed work is outlined in terms of future work on a dendrite-growth model as well as properties of SEI-CEI but added that more planning and experimental design are needed.

Reviewer 4:

The reviewer remarked that there was very little detail in what the future work will involve other than improving what has already done. The reviewer asked what new barriers might show up.

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

Reviewer 1:

The reviewer commented that it is highly relevant as Li-dendrite growth continues to be critical issue for both Li-metal BLI batteries and for Li-ion batteries subjected to extreme fast charge. Also, interfacial impedance at the Li-metal solid electrolyte interface is another critical Li-battery issue.

Reviewer 2:

The reviewer found the project to be highly relevant and directly supports the DOE overall objectives, such as designing Li-ion batteries with low price, high energy density, and excellent cyclability. The reviewer added that low performance and high cost are the main challenges and the present project effectively addresses them.

Reviewer 3:

The reviewer indicated that dendrite growth has become an area of intense DOE interest.

Reviewer 4:

The reviewer wrote that the DOE objective of dendrite-free Li electrodes and delamination-induced performance decay have been addressed to some extent.

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 project team has sufficient financial, computational, and human resources to complete the project in a timely manner.

Reviewer 2:

The reviewer said the resources are sufficient for the work being accomplished.

Reviewer 3:

The reviewer described project resources as okay.

Reviewer 4:

The reviewer stated that at this moment, the resources look sufficient, but added that collaboration with a statistical engineering group will be good to understand the experimental design concept.

Presentation Number: bat310
Presentation Title: Advancing Solid-State Interfaces in Lithium-Ion Batteries
Principal Investigator: Nenad Markovic (Argonne National Laboratory)

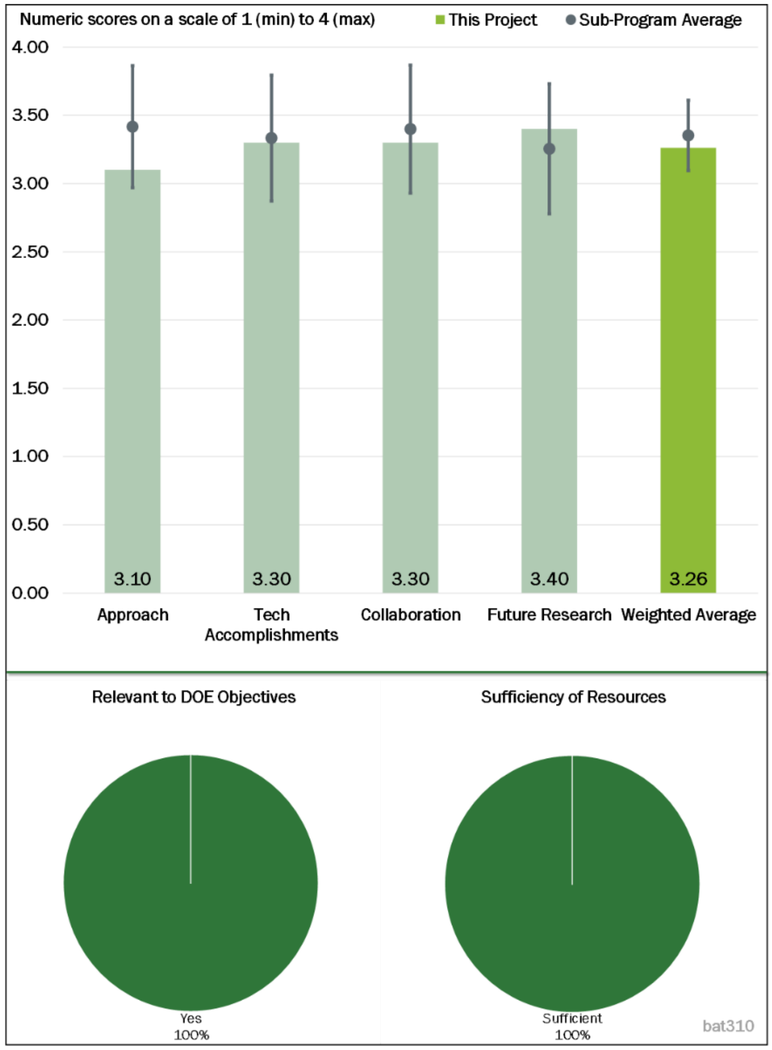

Figure 2-32 – Presentation Number: bat310 Presentation Title: Advancing Solid-State Interfaces in Lithium-Ion Batteries Principal Investigator: Nenad Markovic (Argonne National Laboratory)

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:

The reviewer explained that this project aims to understand the interface between a Li and a solid-state electrolyte, which is very difficult to achieve. The reviewer found as quite convincing the approach of the PI and co-PI of combining the experimental and theoretical methods.

Reviewer 2:

The reviewer observed that the focus of the work has been to develop atomistic models to understand the differences in dopant-dependent surface and interface reactivity. The PIs have shown that by modeling they can provide evidence for a thermodynamic driving force for why niobium (Nb) is different from tantalum (Ta) and Al doping. The reviewer elaborated that the project team was able to show experimental data to support this claim, showing that Li reacts at the surface of the Nb-doped LLZO whereas with Al and Ta there is minimal change. The project has addressed the technical barriers adequately and the experimental and computational work has supported their designs.

Reviewer 3:

The reviewer noted that the PI adopted an integrated approach that involves synthesis, characterization, and theoretical calculations, adding that this is very good. Doping cations with various valences were chosen to improve the ionic conductivity of lLLZO. The improvement was understood with the aid of theoretical calculations and electrochemical characterizations. The reviewer had one minor doubt about the electrochemical method used in this project, which may not be able to probe the bulk.

Reviewer 4:

The reviewer stated that the approach, consisting of both modeling and experiments, is quite comprehensive and sophisticated. However, the reviewer added, it seems quite insufficient in small-scale mechanical characterization, especially in such small dimensions as the thin-film model systems that the team has been working on and will be making.

Reviewer 5:
The reviewer remarked that the project mainly focused on examining the effect of dopants on the stability of LLZO. It also looked at the redox stability of lithium lanthanum titanate (LLTO). The techniques involve growth of single crystals and amorphous films and a suite of characterization tools along with DFT calculations. As previously pointed out, the reviewer stated that the work largely used Li-Li cells and the specification of the electrolyte layer is not provided (thickness and density or residual porosity).

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 overall progress of this project appears to be on track. The project team has done lots of work, including two published papers and one manuscript in preparation.

Reviewer 2:
The reviewer found that some important observations on the reaction of Li plus SSE, and a doping effect have been found. The reviewer noted that a paper was published recently in Advanced Energy Materials.

Reviewer 3:
The reviewer noted that the team's initial milestones have been completed within the allotted time and the next two milestones seem to be in line. One concern the reviewer expressed is that the PIs are using an appropriate experimental setup to distinguish the chemical versus electrochemical reactivity at the interface between the cathode and the electrolyte and the anode and the electrolyte. It was directly clear to the reviewer what loadings were going to be tested, how those would impact performance, and how the surface lithium carbonate would influence their modeling results.

Reviewer 4:
The reviewer replied that the project is either completed or on schedule.

Reviewer 5:
The reviewer noted that the project observed a clear effect of the dopant, in particular Nb. However, the reviewer added, electrochemical data are of limited utility. A very short pulse was applied at two different current densities to a sample with unknown thickness. Testing under more realistic conditions should be undertaken, in particular with much higher capacity throughput. In addition, the reviewer asked what the Nb data mean. The reviewer concluded that if it is due to mixed conductivities, they need to be measured.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found excellent collaboration with computational scientists but added that the project team can be strengthened by more expertise in solid-state electrochemistry.

Reviewer 2:
The reviewer reported that the external collaborators include leading experts at the University of Michigan and Northwestern University.

Reviewer 3:
The reviewer stated that it seems that the project team has been collaborating well between the computational and experimental work. The project team has been receiving samples from a reputable source for making high-quality LLZO pellets. The reviewer suggested that the researchers work as a team to help develop a more

robust mechanism for their oxygen-deficient layer as it would be interesting to locally provide more oxygen on the surface to investigate how that changes the performance.

Reviewer 4:
The reviewer remarked that the project team does not seem to have sufficient expertise in small-scale mechanical testing, especially at the nano-meter length scales that are required for understanding the mechanical behavior of Li-metal, solid electrolyte, and cathode systems.

Reviewer 5:
The reviewer stated no comment.

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 it is great that a full-cell study was proposed.

Reviewer 2:
The reviewer praised the proposed future work as exactly what needs to be done—studying the "real" interphase when the solid electrolyte is coupled with lithium. At the current stage, the reviewer wrote, the study is still only focused on the solid electrolyte itself. But it is critical to move on to the next stage and see how the chemical and electrochemical stability varies in the presence of Li-metal.

Reviewer 3:
The reviewer recommended that the project produce more relevant cycling data to improve the relevance of the surface analysis to impact practice solid-state batteries.

Reviewer 4:
The reviewer observed that the slides mentioned, in response to one of the comments from last year's review, the need for studying the mechanical behavior. However, the reviewer noted, this aspect is not reported in this year's slides and is not mentioned in the future plan. It was unclear to the reviewer from the slides under "In progress" how the team will measure the electrochemical and mechanical behavior of model systems such as thin films of lithium cobalt oxide ($LiCoO_2$) (104)/LLTO (001) & (100)/Substrate, since these structures cannot readily be used for these measurements.

Reviewer 5:
The reviewer thought the project team has so far been able to effectively plan their future work. However, the project team still has yet to show realistic cell performance. The reviewer noted that the project team said that it is next on their list of accomplishments, but when discussing it with them, the project team seemed uncertain as to how to approach the design.

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

Reviewer 1:
The reviewer said this project is highly relevant to the overall DOE objectives.

Reviewer 2:
The reviewer agreed that Li-SSE is a critical research problem.

Reviewer 3:

The reviewer stated that understanding the interface between the Li and solid-state battery is important for designing better solid-state batteries.

Reviewer 4:

The reviewer noted that the project aims at a fundamental understanding of materials and interfaces for all solid-state batteries through a "science-based approach… fast transfer of fundamental knowledge from model to real world systems."

Reviewer 5:

The reviewer explained that ceramic solid-state electrolytes are important for approaching safer batteries. Specifically, LLZO has high ionic conductivity and minimal reactivity at the Li interface. The reviewer found that the work builds upon previous studies and investigates why various dopants have differing performance. Additionally, the PIs understand the role of both of the interfaces and the challenges that they present. They have found that Li symmetric cells show this and are working toward more realistic cells. However, the reviewer added, there are some intrinsic limitations to LLZO, namely the high cost of manufacturing, the brittle nature of the ceramic, and interfacial impedances at both the Li and cathode interfaces. So far, the reviewer concluded, the team has focused on the Li side and a major challenge is going to be on the cathode.

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

Reviewer 1:

The reviewer indicated the resources for this project have been satisfactory, adding that the project team has been able to utilize those resources appropriately.

Reviewer 2:

The reviewer wrote that the project team is applying tools to state-of-the-art problems and the resources are adequate to make progress.

Reviewer 3:

The reviewer agreed that the resources on this project are sufficient to meet the milestones.

Reviewer 4:

The reviewer concluded the project team has all the necessary resources, except for small-scale mechanical characterization of thin films and interfaces.

Reviewer 5:

The reviewer wrote no comment.

Presentation Number: bat311
Presentation Title: Understanding and Mitigating Interfacial Reactivity Between Electrode and Electrolyte
Principal Investigator: Dusan Strmcnik (Argonne National Laboratory)

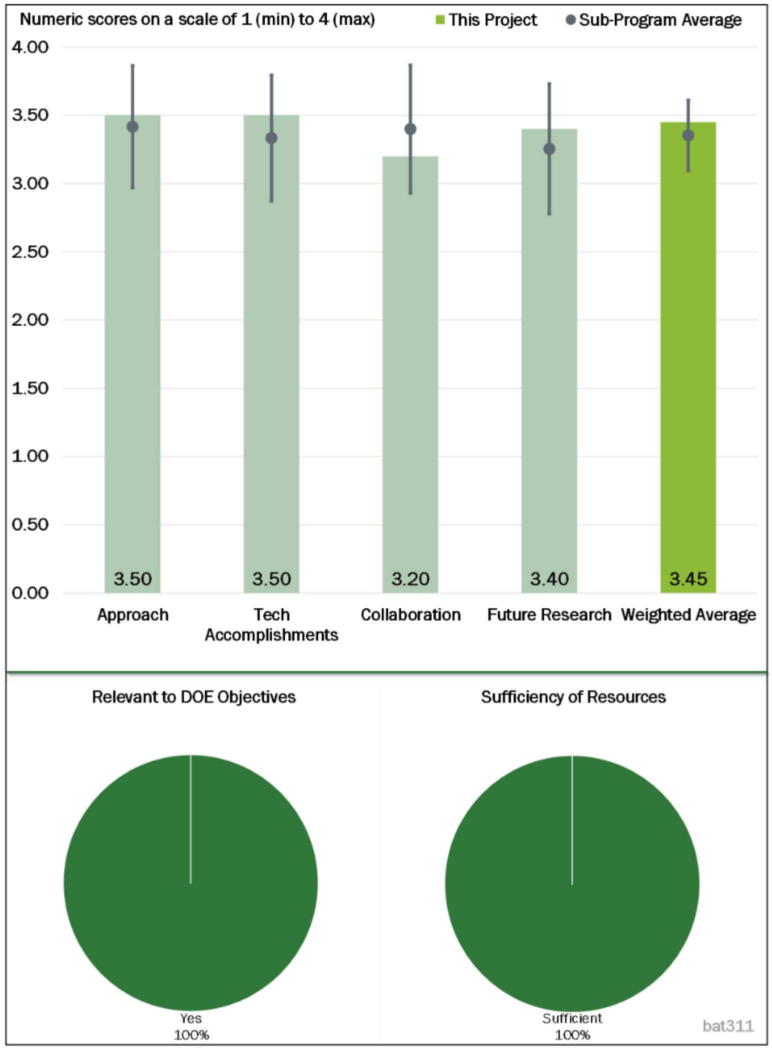

Figure 2-33 – Presentation Number: bat311 Presentation Title: Understanding and Mitigating Interfacial Reactivity Between Electrode and Electrolyte Principal Investigator: Dusan Strmcnik (Argonne National Laboratory)

Presenter

Dusan Strmcnik, 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 replied that the team has put forward a fundamentally motivated, science-based approach, which combines in-situ electrochemistry, a model, well-defined electrode-electrolyte interfaces, and theory and modeling, in order to study degradation mechanisms at the cathode-electrolyte interfaces especially for high-voltage cathodes.

Reviewer 2:

The reviewer praised the approach to the technical work as unique and added it should provide a fundamental basis for understanding decomposition of cathode-electrolyte interfaces. Separating each chemical or electrochemical process through careful selection of materials and precise electrochemistry provides the sort of insight necessary to ultimately select better material sets and addresses the problem of electrolyte design and interface design. The experimental tools are appropriate, the reviewer said, but cautioned that the success of the project will depend on the ability to find suitable model surfaces for study that allow deconvolution at a mechanistic level.

Reviewer 3:

The reviewer commented that one of the strengths of the project so far is the development and adaption of powerful analytical tools (e.g., stationary probe rotating disk electrode [SPRDE] and OEMS) to address the issues associated with the cathode-electrolyte interface at high potential. These types of tools have been very useful in related studies of bulk electrolyte stability and even SEI formation and dynamics.

It was clear to the reviewer that the PIs hope to apply these powerful tools to study the dynamics and evolution of the cathode (electrode-electrolyte interface or EEI in their terms) largely by trying to isolate individual effects one at a time via very careful and extensive studies. The vision is that the work will provide the "endpoints" to battery developers—that is, the range of effects that are possible as the result of each individual parameter variation— so that they can effectively address the technical barriers for high-voltage cathodes. While this make sense at first glance, the reviewer found it questionable about how practical it really is. There are so many variables involved, and most of them are coupled— e.g., solvent degradation may only be seen in the presence of trace acid and high voltage. So, studying the individual components separately with such fidelity but without coupling between components of the problem will get one only so far. Perhaps one of the reasons that simple models have yet to capture the observed complex behavior is that they also fail to include the coupling between parameters. So, for the PIs to bridge the gap between experiment and modeling, the reviewer suggested they will have to do experiments that have coupled effects so that the models can get better.

The reviewer concluded that there is plenty to do here— and the proposed approach is certainly not without value —but the PIs should consider strategic inclusion of experiments with coupled, but controlled, parameters to help produce validation data for model development. Bridging the gap between models and experiment is absolutely necessary to make rapid progress here—there are simply too many parameters (e.g., materials and processing variables) to methodically sort through them one at a time with exceptional experimental rigor.

Reviewer 4:

The reviewer stated that the approach is interesting, as the experimental set-up allows probing of materials directly from electrochemistry. However, it was not clear to the reviewer how the researchers plan to address the possibility of the formation of oligomers or inorganic content upon electrolyte decomposition. Gaseous and liquid products may not be the only species that form.

Reviewer 5:

The reviewer noted that the project aims to address the stability of the cathode materials and the electrolyte, which is very relevant with barriers in batteries. The reviewer added, however, that the approaches to using Pt or Pt-based materials as the model system seem far away from the real material systems.

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:

Despite being only a few months old, the reviewer found that the project has made very notable progress in getting experimental protocols set up, equipment built and calibrated, and initial experiments completed. The reviewer commented that this fast start is probably due to similar work that the group has done on related work on interfaces and bulk material stability, but the current project is benefitting from the depth and experience of this project team. The experimental demonstration that the solvents are largely stable above 5V in the absence of coupled factors is a very significant early result. Despite the broadness of the approach (that is, the uncountable number of variables and parameters that could be studied), the list of milestones is more specific and could probably serve as a reasonable guide to keep the project moving forward at the pace seen so far. The reviewer concluded that comparing the non-fluorinated and fluorinated solvents will be an important result and should be prioritized.

Reviewer 2:

Noting that this is a new project only in its first year, the reviewer indicated that the team has already gotten off to a good start with a comprehensive analysis of the ethylene carbonate (EC) and ethyl methyl carbonate (EMC) based electrolytes using a suite of analytical tools (gas chromatography mass spectroscopy [GC-MS] and integrated coupled plasma mass spectroscopy [ICP-MS]) and established the feasibility of a method to integrate the SPRDE with ICP-MS for organic carbonates. The project is on track for the proposed scientific advances.

Reviewer 3:

The reviewer wrote that the program is new and is taking advantage of infrastructure that is already in place. The progress is appropriate.

Reviewer 4:

Noting that some interesting findings were observed, the reviewer understood that this is a very complicated study and may require more time to have breakthroughs.

Reviewer 5:

The reviewer remarked that as the project has very recently started, there is limited progress to report. The setup of the SPRDE with ICP-MS and OEMS apparatuses appears successful and should lead to very interesting data after validation. Initial reports on metal surfaces show electrochemical trends with the presence of surface oxygen, suggesting that identification of clean and appropriately terminated surfaces relevant to actual cathode materials will be extremely important. Selecting and preparing single-crystal oxide surfaces containing Li^+ should be a target. The reviewer noted that some studies that distinguish between the effects of Li^+ and other cations (i.e., tetrabutylammonium [$TBA^{+]}$]) as well as various anions should be included. While it may be out of the scope of the project, electrochemical atomic force microscopy (AFM) could be useful for correlating local crystal structure with electrochemistry.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer responded that collaboration across the project team is clear, pointing out that this project team has worked successfully together before. There are no concerns here. In the future, the reviewer suggested the project team will need fluorinated solvents from collaborator Zhang, and hopefully there will be no issues when the time comes for the studies to progress to the fluorinated solvents.

Reviewer 2:

The reviewer stated that the project team has a clearly identified collaboration with an ANL scientist for fluorinated electrolytes for this research.

Reviewer 3:

The reviewer said cooperation among the group is appropriate.

Reviewer 4:

As the project just started, the reviewer wrote that collaboration between the two partners has not yet commenced.

Reviewer 5:

The reviewer stated that more collaborators should be identified.

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

Reviewer 1:

The reviewer wrote that the team has clearly identified the tasks, made plans for the required experimental method advancements and model system development to study, and identified clear connections with the theory and computational studies.

Reviewer 2:
The reviewer replied that the proposed future work should be quite interesting if it is possible to deconvolute all of the independent electrochemical phenomena.

Reviewer 3:
The reviewer indicated the focus on metal substrates is understandable in the attempt to use model materials with well-defined surfaces. However, the reviewer added, electrochemistry is surface dependent, so moving toward the metal oxide surfaces is encouraged.

Reviewer 4:
The reviewer commented that the list of milestones lays out a good plan for the future work— there is some specificity in what solvents will be prioritized in the future work in the project. The description of future work later in the presentation, however, was a bit vaguer in that everything was generalized to “electrolyte” and “transition-metal oxide.” The reviewer observed that while it is understood that the project is still early in the “discovery phase”— identifying what reactions and dynamics appear to be the most important—this exploratory part of the project cannot go on in parallel for the full 36 months of the project. The result would be never-ending changes in priorities of what the focus is. The reviewer’s suggestion is for the PIs to clarify soon which reactions and dynamics appear to be the most important and then focus the future work on those priorities.

Reviewer 5:
The reviewer remarked that some proposed studies are high risk.

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

Reviewer 1:
The reviewer affirmed this project is clearly aligned with the objectives to advance the fundamental understanding of high-voltage cathode and electrolyte-interface degradation and thereby addresses some of the key barriers to enhanced performance, life, and safety for next-generation Li-ion batteries.

Reviewer 2:
Noting that specific goals for DOE VTO will require a better understanding of interfacial reactions, dynamics, and evolution at the cathode-electrolyte interface at high voltages (greater than 4.5V), the reviewer found that this project directly supports that R&D need.

Reviewer 3:
The reviewer replied that battery-material degradation is relevant to DOE’s objectives.

Reviewer 4:
The reviewer indicated that understanding of interfaces is important and will advance the field.

Reviewer 5:
The reviewer suggested that this project should address the need to understand decomposition mechanistically at cathode-electrolyte interfaces, adding that impacts include better design of interfaces to promote the safety and cycle life of cathodes.

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 team is well placed with the advanced and state-of-the-art experimental, analytical tools, and computational resources for successful accomplishment of this project.

Reviewer 2:
The reviewer said resources are sufficient for the proposed research.

Reviewer 3:
The reviewer replied the resources for this project are sufficient.

Reviewer 4:
The reviewer commented that the resources allocated to the project are reasonable given the scope, but only if the PIs prioritize the new opportunities that develop during the course of the work and maintain a focus on the highest priority EEI phenomena.

Reviewer 5:
The reviewer had no comment.

Presentation Number: bat312
Presentation Title: Advanced Lithium-Ion Battery Technology: High-Voltage Electrolyte
Principal Investigator: Joe Sunstrom (Daikin America)

Presenter
Joe Sunstrom, Daikin America

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

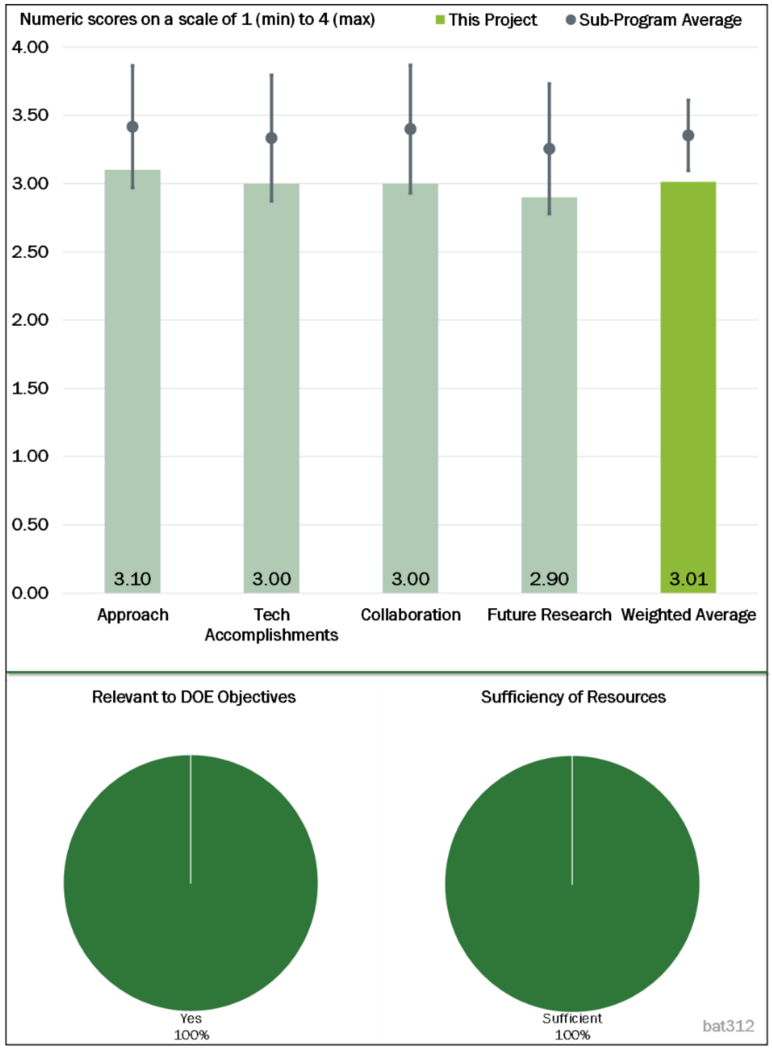

Figure 2-34 – Presentation Number: bat312 Presentation Title: Advanced Lithium-Ion Battery Technology: High-Voltage Electrolyte Principal Investigator: Joe Sunstrom (Daikin America)

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 research work has been performing well along with the clear objectives and timeline. The reviewer added that the technical barriers were determined for the evaluation of SEI film thickness and composition, and milestone in Year 2 was focusing on these issues and coming up with possible and comprehensive solutions.

Reviewer 2:
The reviewer commented that the value of identifying a stable high-voltage electrolyte for Li-ion batteries cannot be overstated. The project continued to take a systematic approach to identifying the role of fluorinated electrolytes on cell performance.

Reviewer 3:
The reviewer remarked that the Daikin team demonstrated the effectiveness of fluorinated additives to improve electrolytes for high-voltage Li-ion cells. They had a sound approach to understanding the electrolyte-failure mechanism by analyzing the passivation film on the high-voltage cathode surface.

Reviewer 4:
It was unclear to the reviewer why the project team chose to utilize anode-limited cells while the industry standard is to use cathode-limited cells. Anode-limited cells frequently encounter problems associated with Li plating. In addition, the project team should not utilize a since cell type for charging to different potentials. The reviewer stated that different cells with optimal balancing should be used for the different voltages since the capacity of the cathode will increase with increased voltage.

Reviewer 5:

The reviewer noted the approach is to propose electrolyte-solvent systems through a design of experiments for high-voltage battery systems with increased cycle life; the experimental approach also includes additive exploration. This work also increases a characterization of the SEI in order to better understand the failure mechanism. Part of the projects team's design was to have an anode-limited cell. This reviewer wrote that this seems problematic because it will likely result in Li plating on the graphite at high-voltage charging.

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 good progress was achieved, adding that the team was able to identify an electrolyte that allows an NCA cathode to cycle at 4.6V.

Reviewer 2:

The reviewer said the milestone in Year 2 was mostly completed with the progress in understanding of SEI composition and thickness. The technical issues were also mentioned and resolved.

Reviewer 3:

The reviewer wrote that preliminary analysis of baseline and fluorinated electrolytes provided good insight on the composition and thickness of the passivation film. The reviewer recommended that the project team should continue to correlate the composition and thickness as a function charge of cut-off voltage and propose a failure mechanism.

Reviewer 4:

The reviewer remarked that project team is on the third and last year of the project, and it is not clear that it will meet the milestone of 400-1000 cycles at 4.6V. On Slide 5, it seems there is 11% capacity fade for 200 cycles at 4.6V. An understanding of the failure mechanism is not complete. For example, SEI characterization as a function of applied voltage has not yet been completed. The reviewer added it would also be helpful to characterize via impedance spectroscopy.

Reviewer 5:

The reviewer stated it was not clear if the project team has achieved the original goals. The original goals stated performance for 300-100 cycles, but the current report shows only 200 cycles. It was also unclear to the reviewer what level of understanding the project team has developed on failure modes. The reviewer also said some data related to cathode-surface films were presented, but the link-to-failure mode mechanism was unclear.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer observed that the research group collaborated with some partners (from different institutions) in characterization of SEI layer (composition and thickness). This group gets the advantage from the expertise of advanced characterization techniques (focused ion beam [FIB]-SEM and time-of-flight [(TOF]-SIMS).

Reviewer 2:

The reviewer noted the project team includes Physical Electronics (PHI) of Minneapolis, the University of Texas at Dallas, and Evans Analytical Group, adding that it seems that all project team members are contributing to this effort.

Reviewer 3:

The reviewer remarked that the project the team is collaborating with the University of Texas at Dallas.

Reviewer 4:
While there was clear collaboration between the lead and PHI related to Auger and SIMS, the reviewer said data analysis and clarity of an understanding of the benefits of the experiments were unclear. Additionally, the contribution of the other partners was unclear to the reviewer.

Reviewer 5:
The reviewer said project team collaboration seemed to consist of subcontracting with commercial partners to provide analytical services.

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 wrote that the project has effectively planned its future work in an obvious manner by determining the goal and also considering barriers to the realization of the proposed technology. The deliverables will be 30 NMC-532 graphite cells with the best practice of a fluorinated electrolyte.

Reviewer 2:
The reviewer noted that the project is ending this year and added that plans for the remainder of FY 2019 are well planned.

Reviewer 3:
The reviewer commented that the project is in its last year, so it made limited comments about next steps.

Reviewer 4:
The reviewer observed that the project team commented on a plan to submit interim cells to the DOE for analysis, but other future plans were unclear. Comments related to additional surface analysis were made, but the goal and benefit of the analyses were unclear.

Reviewer 5:
The reviewer remarked that the project team did not propose future research in writing but mentioned that work will continue on proposing a failure mechanism, albeit with little details.

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

Reviewer 1:
The reviewer said the project is highly relevant but added that identification of a high-voltage electrolyte would be a significant advantage.

Reviewer 2:
As clearly stated in the performance objectives, the reviewer responded that the project has been focusing on understanding of cell failure operating at high voltage, which suggests a new electrolyte and additives to achieve safe, long-term cycling (300-1,000 cycles). The reviewer agreed that these objectives fall into the DOE VTO mission in developing high-energy Li-ion batteries.

Reviewer 3:
The reviewer stated that having a stable, high-voltage electrolyte can improve energy density of Li-ion batteries, assuming that high-capacity electrodes can be selected. This higher energy density, in turn, will lower battery cost, based on dollars per kilowatt-hour.

Reviewer 4:
The reviewer wrote that understanding the electrolyte-failure mechanism is key to improved, high-voltage Li-ion cell performance.

Reviewer 5:
The reviewer indicated that the development of electrolytes with stable performance at high voltage (greater than 4.5V) is important to DOE objectives. The electrolyte formulations developed within the project show promise to assist in obtaining this goal. It was unclear to the reviewer how the electrolyte formulations affect the cost of cell production.

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

Reviewer 1:
The reviewer concluded the resources are enough to cover the milestones of the project in a timely fashion. The estimated expense for 3 years (2017-2019) is around $1,681,000 (versus the whole budget of $1,826,895).

Reviewer 2:
The reviewer said the resources allocated to the project are sufficient.

Reviewer 3:
The reviewer replied resources are appropriate.

Reviewer 4:
The reviewer commented that a stable, high-voltage electrolyte is an enabler for high-energy-density cells and suggested that DOE should develop a concerted effort for a stable, high-voltage electrolyte.

Reviewer 5:
The project team has sufficient resources to complete the tasks, the reviewer wrote, but added that one area that may be helpful to improve understanding of the SEI and its growth is impedance spectroscopy.

Presentation Number: bat319
Presentation Title: Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte
Principal Investigator: Shirley Meng (University of California at San Diego)

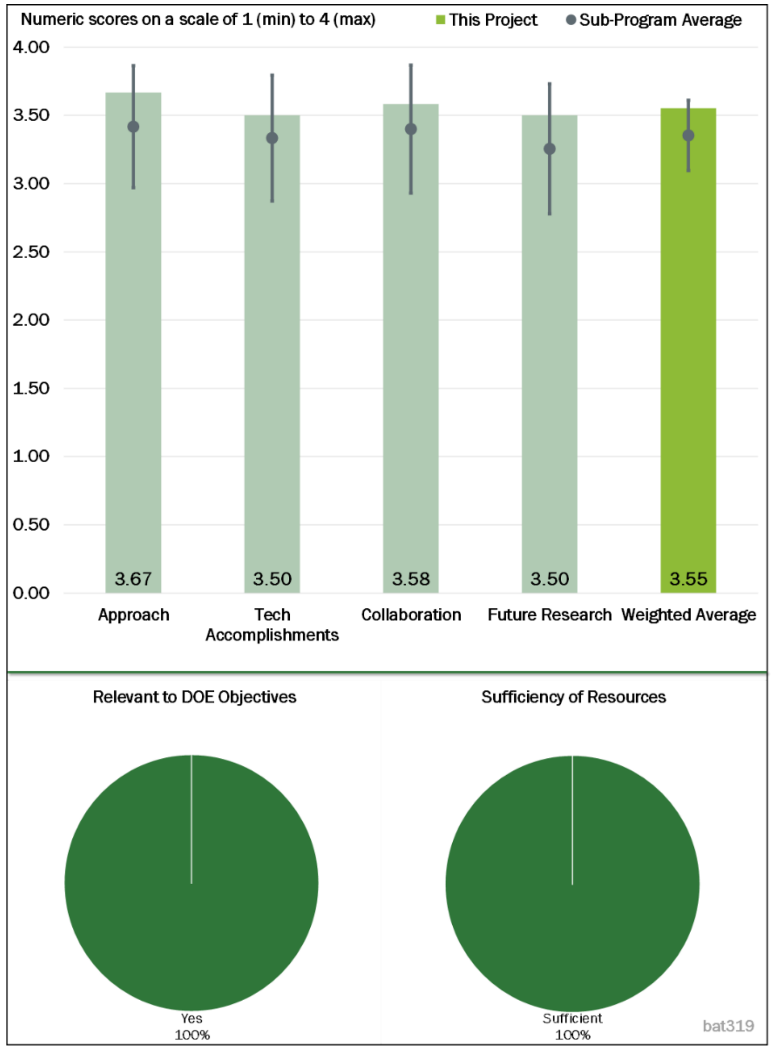

Figure 2-35 – Presentation Number: bat319 Presentation Title: Advanced Microscopy and Spectroscopy for Probing and Optimizing Electrode-Electrolyte Principal Investigator: Shirley Meng (University of California at San Diego)

Presenter

Shirley Meng, University of California at San Diego

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 commented that the project team has demonstrated several technical accomplishments and progress in the overall project. The diagnostic techniques including HRTEM and electron diffraction (ED), in-situ neutron diffraction, and operando Bragg-coherent diffractive imaging (BCDI) (reported before) combined with DFT calculation were applied appropriately to address the role of defects and strain in the voltage-decay issue in Li-excess NMC cathode materials. The reviewer concluded the approach is appropriate and well demonstrated to provide a further understanding of the structure-performance degradation relationship for Li-excess NMC cathode materials.

Reviewer 2:

The reviewer noted that this project has combined STEM and EELS, operando BCDI, and DFT computation to probe anion redox and oxygen evolution in Li-excess NMC cathode materials. The project has also used in-situ neutron diffraction to characterize the bulk material properties. The approach has successfully elucidated the molecular mechanism of anion oxidation and identified the role of defects and strain in the voltage-decay issue. Overall, the reviewer said, the proposed approach can well address the technical barriers.

Reviewer 3:

The reviewer found that the research project has been performing well with clear objectives and timeline. The technical barriers were sharply focused by using advanced microscopy and spectroscopy to study Li-rich cathode materials. Mitigation strategies were proposed to optimize the anion activities in Li-excess NMC-cathode materials by mild heat treatment.

The reviewer added that the milestone in FY 2019 has been fruitful, with an innovative solution to obtaining good performance of Li-rich layered oxide (LRLO) (gas–solid interface reaction [GSIR] and electrolyte benchmark) and an interesting cause and solution for Li-metal problems.

The reviewer wanted to know how many cycles could be obtained here in the high concentration ether based for electrolyte Next, the reviewer asked if the PI could explain in more detail about the assistance of an artificial SEI and the 3-D current collector. Lastly, the reviewer questioned if they are practical for a real application.

Reviewer 4:

The reviewer said that characterization techniques continue to be important tools in understanding battery-system dynamics.

Reviewer 5:

The reviewer remarked that the PI is highly innovative in developing spectroscopy tools to answer chemistry questions. One concern from the reviewer was whether single-particle analysis will be sufficient to generalize results. It has been established that there is quite a bit of particle-to-particle heterogeneity in porous electrodes, so the reviewer advised picking several particles to ensure representative behavior (perhaps this was done, but the reviewer saw no evidence of it in the presentation).

Reviewer 6:

The reviewer wrote that project team has developed several complementary measurement techniques to investigate both the Li-rich, layered-oxide positive and Li-metal negative electrodes. However, a comprehensive and coherent understanding of these materials is still illusive. For example, the connection between strain and degradation was unclear to the reviewer and is not part of the future plan.

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 project team provided several technical accomplishments and progress against milestones. The team has responded well to the questions raised from reviewers in the previous year. DFT calculations were applied to understand the influence of defect generation on the structural meta-stability and voltage decay. There is an improvement in cycle stability of the modified LRLO cathode with the new electrolyte, and the reviewer commented that following the results will be interesting.

Reviewer 2:

The reviewer wrote that the HRTEM and ED characterization results demonstrate the partial recovery of structure ordering along the layer-stacking direction. Both the DFT calculations and electrochemical testing together with the neutron diffraction support the role of heat treatment in structure and voltage recovery. The LRLO activated by the gas-solid interface reaction can enhance its discharge capacity but still cannot effectively suppress the capacity fade. It still was not clear to the reviewer how the LiBOB additives in the carbonate electrolyte influence the cathode-electrolyte interface, which deserves further investigation. The plating and stripping of Li in engineered electrolytes require further investigation. Milestones have been met. The reviewer concluded the technical accomplishments made in the project are satisfactory.

Reviewer 3:

The reviewer stated that the PI gained insight into structural causes of cathode lost capacity. The proposed remedy of heat treatment is interesting but seems problematic to use in practice (except perhaps for a solid-state battery that can be heated to 300°C). The reviewer commented that the practicality problem was noted in last year's review and the response was that heat treatment idea might give insight, to which the reviewer asked what the insight is and what other strategies are available. The reviewer added that some of the other accomplishments seemed disconnected from the original approach of using spectroscopy to probe the system but nevertheless yielded some insights. The group seems on track in their milestones and in publications.

Reviewer 4:
The reviewer replied that the milestone in the final ear is mostly on track with the overall objectives of the proposed research. The remaining challenges were mentioned with the explanation how the energy density of batteries fades and interaction between novel electrolyte and modified electrode should be explored when cycling at high voltage. Progress in the project will involve confronting these challenges.

Reviewer 5:
The reviewer said milestones are on track and completed as appropriate for the project timeline.

Reviewer 6:
The reviewer suggested that the project team should also report the high C-rate results of the LRLO-positive electrode materials.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that the research group largely collaborated with some partners (from different institutions) in performing the project. The collaboration and interaction help to profit from the expertise of different knowledge and skills to get through the technical barriers and come up with the innovative breakthrough.

Reviewer 2:
The reviewer wrote that collaboration with partners of ORNL, LBNL, ANL, Irvine Materials Research Institute (IMRI), and the Chinese Academy of Sciences is effective in the project.

Reviewer 3:
The reviewer found that publications and research point to good collaboration across the project team.

Reviewer 4:
The reviewer replied that the project team has developed power-characterization tools that are generally applicable to solving a wide range of problems in electrochemical energy storage.

Reviewer 5:
The reviewer responded that the collaboration seemed good to the reviewer. Additional collaboration between the project team and the industrial partner could be helpful to make this work more effectively.

Reviewer 6:
The reviewer commented that collaborators for use of diagnostic tools were explicitly noted and appear to be adequate. The reviewer added that more collaboration with materials-focused groups might help provide additional insight in how to overcome degradation of active material.

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 targets have been effective planned to deeply characterize anion evolution on a modified Li-excess NMC cathode, atomic-scale interaction between novel electrolyte-modified electrode, and

finally SEI layer on electrochemically deposited Li metal. The reviewer added that use of advanced techniques to probe/diagnostic is critical.

Reviewer 2:

The reviewer indicated that proposed future research logically follows on past work and seems to be logically built on identified challenges.

Reviewer 3:

The future research plan appeared to the reviewer to be on track with the overall objectives of the proposed research. XPS and DEMS characterization will be useful for this proposed work. Additionally, to the reviewer, the result of the voltage-recovery behavior by thermal heat treatment is more interesting. Although this approach is not that practical for direct applications in industrial level (as mentioned in the poster presentation), the fundamental mechanism of the behavior is worthwhile to study more. The question is how to transfer this thermal recovery to the electrochemical method in the cell level, which is a more practical approach. For this, the reviewer suggested that more effort to make a better understanding and build a bridge between thermal treatment to the electrochemical recovery behavior of LRLO should be made in future work. Although the reviewer understood its difficulty, it will be great if the project team can continue this work to get a further understanding of the thermal recovery behavior and make this work more practically meaningful.

Reviewer 4:

The reviewer commented that proposed work will lead to additional information— and more detail and thought on how this information will lead to mitigation strategies would be welcome.

Reviewer 5:

The reviewer wrote that the proposed future research is reliable to address remaining challenges. In addition to the proposed techniques, the reviewer suggested consideration of TOF-SIMS and synchrotron XAS.

Reviewer 6:

The reviewer remarked that it is unclear why some of the powerful and seemingly useful tools such as BCDI and neutron diffraction are not considered in the future plan for investigating LRLO and Li-metal electrodes.

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

Reviewer 1:

The reviewer found that this project well supports the overall DOE objectives, adding that the enhanced understanding through this program will be helpful for the development of high-energy-density Li batteries.

Reviewer 2:

As obviously stated in the performance objectives, the reviewer wrote, the project has been focusing on the advanced techniques using microscopy and spectroscopy to probe, understand, optimize, and provide the essential information related to Li-excess, TM oxide cathode materials. The findings and knowledge provided will have critical importance for enabling a major breakthrough in practical development of a high-voltage and high-energy density cathode material using Li-excess TM oxides.

Reviewer 3:

The reviewer indicated that the project fully supports the DOE objectives for diagnosing the high-energy cathodes and Li-metal anode.

Reviewer 4:

The reviewer remarked that the development of improved battery technologies will require considerable understanding of system performance within the internal components of the battery systems. The interface between the electrode and electrolyte being especially important to the ion-transfer kinetics and reaction reversibility. The reviewer concluded that the creation of tools to increase that understand is important to industry development and advancement.

Reviewer 5:
Both the LRLO and Li-metal electrodes are important to reaching DOE's Battery500 goals.

Reviewer 6:
The reviewer wrote that this work, if successful, will contribute to increasing energy density of Li-ion cells through the use of higher voltage cathodes.

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

Reviewer 1:
The reviewer described as an appropriate amount of resources assigned to this project to achieve the stated milestones in a timely manner.

Reviewer 2:
The reviewer wrote the project team has ample resources.

Reviewer 3:
The reviewer said the resources are enough to cover the milestones of the project until January 2020.

Reviewer 4:
The reviewer replied the resources for the project are sufficient to achieve the milestones in a timely fashion.

Reviewer 5:
The reviewer agreed that research funds seem sufficient to support the work for this project team.

Reviewer 6:
The reviewer commented that resources are adequate for achieving the expected insights but added that additional collaborations outside the current circle of partners might leverage these resources to better effect.

Presentation Number: bat321
Presentation Title: Development of Ion-Conducting Inorganic Nanofibers and Polymers
Principal Investigator: Nianqiang Wu (West Virginia University)

Presenter
Nianqiang Wu, West Virginia University

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

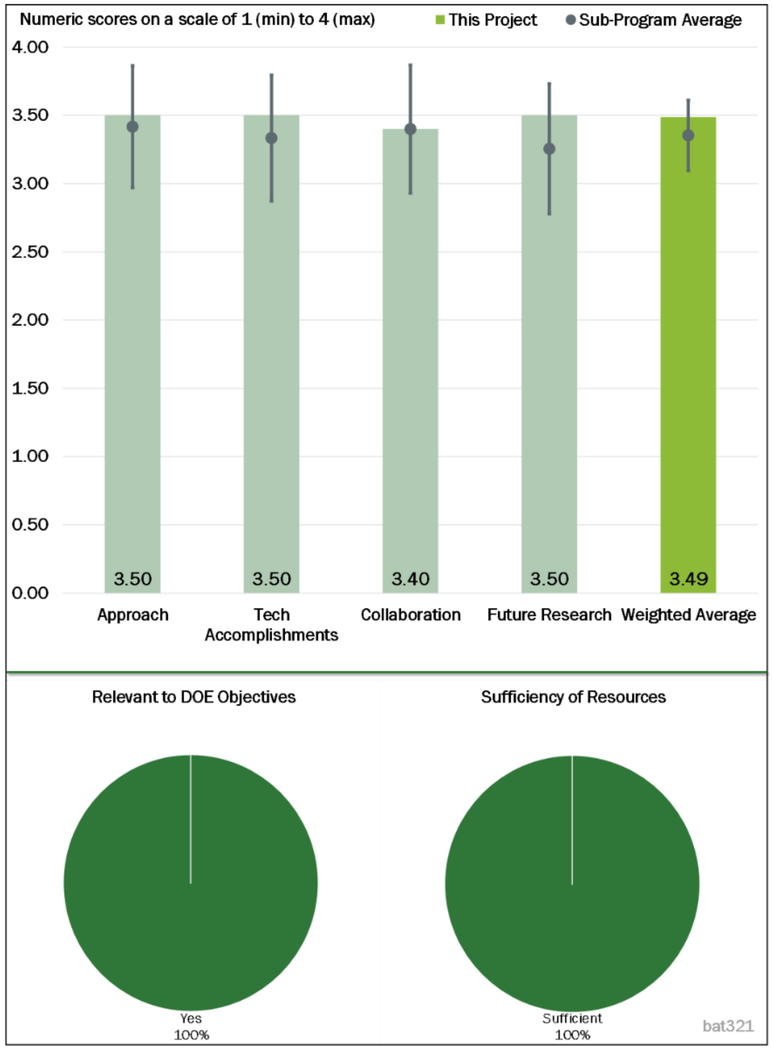

Figure 2-36 – Presentation Number: bat321 Presentation Title: Development of Ion-Conducting Inorganic Nanofibers and Polymers Principal Investigator: Nianqiang Wu (West Virginia University)

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 commented that the work shows good progress toward developing ionic-conducting materials with good ionic conductivity and mechanical properties. Some of the materials appear not to be stable versus Li. An electrochemical impedance spectroscopy (EIS) measurement at time intervals would be helpful to confirm stability. Very good cycling data are shown. The loading of electrode materials in terms mAh /cm^2 or g/cm^2 of electrode material should be listed on the cycling data to determine if the performance has been achieved under meaningful conditions.

Reviewer 2:
The reviewer agreed that the research project has been performing well along with the clear objectives and achievable products following the timeline. The technical barriers were also mentioned and the project team came up with a new concept of polymer configurations and modified ceramic fillers.

Reviewer 3:
The reviewer noted that several approaches have been proposed to address the low conductivity and stability issues of electrolytes in solid-state batteries. Current results demonstrate the effectiveness of these approaches.

Reviewer 4:
The reviewer commented that the PI aims to improve the ionic conductivity and mechanical strength of a solid polymer electrolyte by adding plastic salts and cross-linking Lithium bis(fluorosulfonyl)imide (LisTFSI) and polyethylene(glycol)diacrylate (PEGDA). Such approaches make sense and the PI succeeded in making desired improvements. The PI also aims to improve the ionic conductivity, decrease the interfacial resistance,

and increase the transference number by introducing silane-grafting. The reviewer indicated this is also a good approach as verified by the improved ion-conducting properties of the silane-grafted composite electrolyte. The improved performance is further validated in full-cell testing.

Reviewer 5:

The reviewer wrote that the proposed approach successfully mitigates problems with solid electrolytes or polymer electrolytes such as PEO or PVDF-LiTFSI. Improved performance has been demonstrated. However, the reviewer noted, application for high-voltage and high-capacity aggressive cathodes is likely to be problematic and limits impact of this 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 said significant accomplishments have been made in all approaches.

Reviewer 2:

The reviewer commented that the program appears to have accomplished many of the planned milestones such as improved conductivity and mechanical properties. The reviewer added that Indications of the loading will be useful to fully appreciate the progress made on these systems.

Reviewer 3:

The reviewer indicated that good progress has been made, elaborating that three types of polymer matrix have been tried and two of them (PEGDA+PETA and PEGDA+LisTFSI) demonstrated improved performance. Two types of composite electrolytes (s@LLAZO+PEGDA+LiTFSI, and LPO-LLATO/PVDF-HFP/LiTFSI) have been synthesized and optimized. Full cells using either $LiFePO_4$ as cathode or sulfur as cathode have been fabricated and tested.

Reviewer 4:

The reviewer affirmed that milestones in the final year are mostly on track with the overall objectives of the proposed research. The remained challenges were mentioned, and some suggestions were raised for expanding the research.

Reviewer 5:

The reviewer found good progress toward meeting milestones and demonstrating Li metal versus LFP or S cathodes. However, the reviewer said that stability toward high voltage and high-capacity NMC is not clear. The reviewer asked what the path is to achieve high-energy density and go beyond LFP.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer observed that the research group collaborated with some partners (from national and international institutions) in performing the project. The reviewer added that the collaboration and interaction help the project profit from the expertise of different knowledge and skills to get through the technical barriers and come up with the innovative breakthrough.

Reviewer 2:

Noting that the collaborators include North Carolina State University and the Quzhou University of China, the reviewer wrote that the list could be expanded.

Reviewer 3:

The reviewer found excellent collaboration within the project team. However, the reviewer said it is not clear what information the modeling partner has provided to the project.

Reviewer 4:
The reviewer said it appears from results that collaborations are working, but if more details are provided as to origin of each result, it would enable a more thorough evaluation.

Reviewer 5:
no comment.

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 the future targets have been effectively planned to optimize the interface between the electrolyte and the electrode, decrease interface resistance, which has significant effect on the performance of full-cell batteries. The challenges in finding the grafting agent providing high ionic conductivity and optimizing the ionic conductivity of polymer membrane will be confronted.

Reviewer 2:
The reviewer concluded that the optimization of the electrolyte structure is expected to further improve the performance.

Reviewer 3:
The reviewer wrote the proposed future research is appropriate.

Reviewer 4:
The reviewer explained that the PI proposes to try different grafting agents in the future, which is sensible. The PI also proposes to modify the ceramic nanofiber surface, which sounds challenging. The proposed work "optimizing the ionic conductivity of composite electrolyte" sounds general because the composite electrolyte is indeed complicated, and it is better to be specific about the direction of optimization. The reviewer concluded that the proposed future work on battery fabrication looks reasonable.

Reviewer 5:
The reviewer concluded that the proposed research does not address compatibility with high voltage/capacity aggressive cathodes.

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

Reviewer 1:
The reviewer affirmed that the project strongly supports the overall DOE objectives, adding that a good solid polymer electrolyte is very important for beyond Li-ion batteries.

Reviewer 2:
The reviewer found the project has been focusing on the development of solid-state composite polymer electrolyte providing higher ionic conductivity, improved mechanical strength and better stability than PEO-based polymer electrolyte. The research term is attached to the DOE objectives in shifting to the use of solid-state electrolyte for safety concerns in the electric vehicles and electronic portable devices as well.

Reviewer 3:
The reviewer noted that most of the research is focused on toward developing materials to enable high energy cells of interest to DOE mission.

Reviewer 4:

The reviewer commented that Lithium metal batteries will improve energy density if ever they are proved to be safe.

Reviewer 5:

The reviewer responded that better electrolyte for solid electrolyte battery is needed.

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 resources are well managed and results are disseminated through publications.

Reviewer 2:

The reviewer commented that the resources are sufficient to meet the objectives.

Reviewer 3:

The reviewer replied that resources on this project are sufficient to meet the milestones.

Reviewer 4:

The reviewer replied that the resource is enough to cover the milestones of the project until the end of FY 2019.

Reviewer 5:

The reviewer wrote no comment.

Presentation Number: bat322
Presentation Title: High Conductivity and Flexible Hybrid Solid-State Electrolyte
Principal Investigator: Eric Wachsman (University of Maryland)

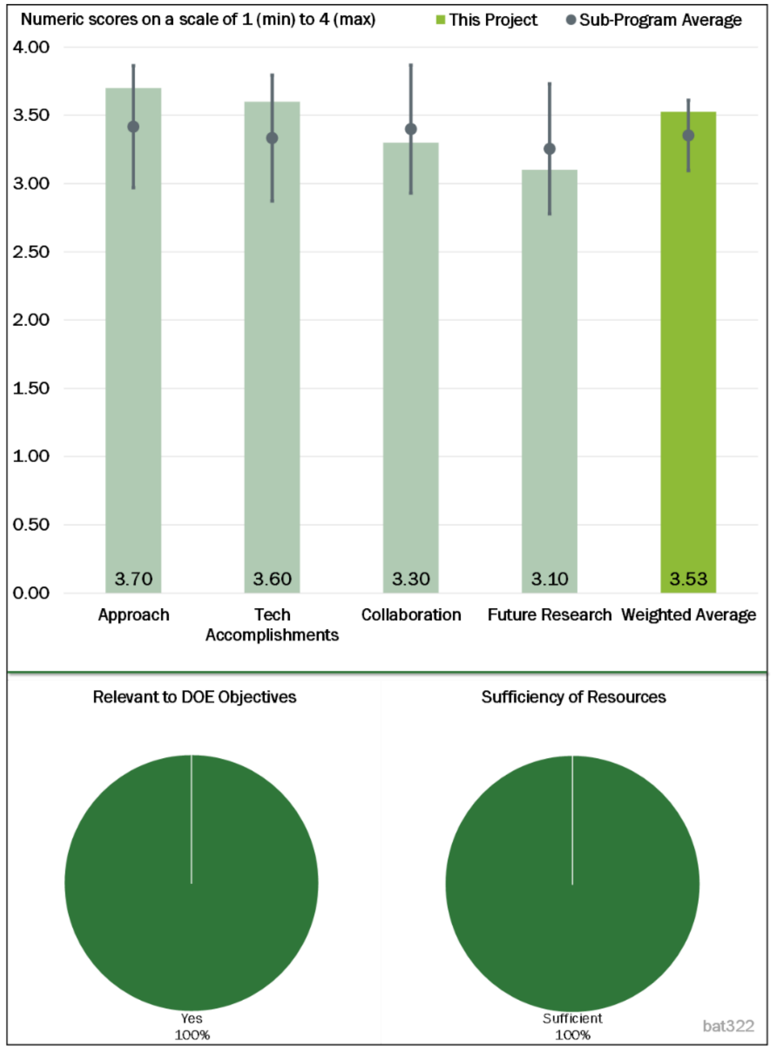

Figure 2-37 – Presentation Number: bat322 Presentation Title: High Conductivity and Flexible Hybrid Solid-State Electrolyte Principal Investigator: Eric Wachsman (University of Maryland)

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 found that the project team clearly understands the barriers confronting a Li-metal battery and attempts to address them in this effort. The reviewer added that the project focuses on a major concern, namely, a high-conductivity, low-internal impedance, solid-state electrolyte.

Reviewer 2:
The reviewer explained that the technical barriers for an inorganic solid-state electrolyte (LLZO), such as low Li-ion conductivity, high interfacial impedance, Li-metal nucleation and growth at the crystal defect site etc., are well addressed by this project. The reviewer elaborated that to achieve the project objectives, such as development of solid-state Li-S batteries exhibiting energy density of approximately 450 Wh/kg for 500 cycles, the approach involves fabricating hybrid flexible solid-state electrolyte composites comprised of inorganic garnet fibers homogeneously dispersed in the polymer matrix. Identification and fabrication of the optimized architecture of hybrid (SSE to achieve high Li-ionic conductivity and mechanical strength led by theoretical calculation are highly promising approaches.

Reviewer 3:
The reviewer replied that the project is nearing completion at the end of FY 2019, and the approach that has been employed over the last 2 plus years has been fine. The combined experimental and theoretical team has been able to overcome a few technical barriers and has positioned themselves to be successful with the final milestone to demonstrate a 450Wh/kg Li-S cell with the thin SSE that has been developed. Whether or not they are successful in this demonstration remains to be seen, but the approach to getting to this point has been more than acceptable. For the most part, the reviewer concluded, the right experiments and calculations have been done along the way.

Reviewer 4:

The reviewer stated that the approach is to develop a high-conductivity (greater than 0.5 mS/cm), flexible, low-interfacial impedance garnet-organic hybrid electrolyte based on garnet nanofibers in order to enable the use of Li-metal anodes and to increase the cell's energy density.

Reviewer 5:

The reviewer described the approach as novel and potentially manufacturable.

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 that excellent results were achieved, adding that the project team's research has resulted in significant knowledge advancement in the area of solid-state electrolytes.

Reviewer 2:

The reviewer concluded that the PI's team made great progress in fundamental understanding of nucleation and growth of Li-metal inside the garnet structure. The reviewer explained that the PI correctly addresses the effects of over-potential or current density and potential gradient on the critical crystallite size and nucleation barrier. In addition, the effect of defects on electronic conductivity has been determined by first-principle's calculation. It will be a great achievement if the PI is able to determine the nucleation barrier at different defect sites using first-principle's calculation or fundamental thermodynamic nucleation theory. Use of a hybrid electrolyte as proposed by the PI could suppress the nucleation and growth of Li metal and could be realized as a suitable SSE for Li-metal batteries. The PI's team also fabricated Li-S full cell to achieve the targeted energy density utilizing high S- loaded S@graphene in carbonized wood as the cathode and a hybrid SSE.

Reviewer 3:

The reviewer said that while it might have been nice to already have some preliminary Li-S full-cell capacity and cycling data at this point (instead of just symmetrical Li-metal cycling to 500 cycles), the progress has been significant up to this point, and the team will have a reasonable chance to demonstrate the 450 Wh/Kg milestone by the end of the project. The reviewer suggested that what might "get lost in the shuffle" at the end of the project is the very nice modeling and simulation results on Li-metal deposition in the pores of the SSE material completed in FY 2019. These results are very nice and will be helpful to many other efforts to suppress or otherwise control dendrites with Li-metal use. Overall, the progress has not been overwhelming—for example, the data presented on the Li-metal symmetrical cycling were sort of bare minimum and were not completely convincing that dendrites would not be observed in other trials and/or under other conditions. However, the reviewer concluded, the progress and accomplishments have been steady and in the right direction. There is one big milestone to go before the end of the project.

Reviewer 4:

The reviewer wrote the accomplishments are very impressive in terms of avoiding dendrites at 3 mA/cm^2. The reviewer added that the focus on small flaws does not address the fact that a glass still passes dendrites and asked what the right way to think about this is.

Reviewer 5:

The reviewer noted that the project goal is 450 Wh/kg and 500 cycles for Li-S cells, but only 6 months remain in the project and no full cell performance data are presented. A Li-S cell has been fabricated and test results were provided for only a single cycle. The project team has demonstrated 17 mAh/cm^2 for the sulfur cathode, but the volumetric loading is not reported, which will impact the cell's energy density.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted that the team is comprised of experimental and computational researchers, who have solid background in solid-state physics, materials science, and electrochemical science, and has access to phenomenal facilities to understand the fundamental key barriers and make innovative solutions for solid-state batteries.

Reviewer 2:
The reviewer concluded that coordination and collaboration have been fine across the group. The publications could have been more "collaborative" in their author lists— but this "metric" is not always an accurate reflection of the actual collaboration and more a result of what journals are willing to publish. From the presentation, it became clearer to the reviewer that collaboration has been very good on this project.

Reviewer 3:
The reviewer observed that researchers at the University of Maryland and University of Calgary are all contributing to the project.

Reviewer 4:
The reviewer noted that there is collaboration with Professor V. Thangadurai (co-inventor of garnet).

Reviewer 5:
The reviewer suggested the project would benefit by a collaboration with industry.

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

Reviewer 1:
The reviewer stated that the proposed future efforts are headed in the right direction, adding that the project will use the knowledge gained in solid-state batteries to demonstrate a Li-S cell.

Reviewer 2:
The reviewer indicated that future research mainly focuses on the integration of computational and experimental research and the development of the full Li-S cells utilizing developed hybrid SSE to achieve the targeted energy density of 450 Wh/kg. The reviewer concluded that a fundamental understanding of Li-ion diffusivity and electronic conductivity led by computational research and development of mitigation strategies will definitely move SSE research forward.

Reviewer 3:
The reviewer remarked that with so little time left in the project before it ends, the proposed future research is very limited— mostly to finish the Li-S full-cell test and determine if the 450 Wh/kg metric can be met. It was not so clear to the reviewer what, if anything, would be done with the mixed ionic-electronic conductor material fabricated with carbon nanotubes. The reviewer asked if this was just a spin-off of the effort or if this S-impregnated material will in anyway be used in the final Li-S milestone. The reviewer concluded that a little clarity on what would and would not be part of the final testing would have helped a bit.

Reviewer 4:
The reviewer wrote that the proposed work states that the project team will demonstrate Li-S cells with 450 Wh/kg and validate computational and experimental results, but the path to meeting these goals was not provided. As the electrode loading increases, the reviewer wrote, it will be more difficult to access the active material. Only single-cycle sulfur cathodes have been included in the presentation.

Reviewer 5:
The reviewer stated the proposed future research is too vague.

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

Reviewer 1:
The reviewer found that the work in this project clearly is aligned with DOE goals to develop and characterize the performance of high-capacity cells (e.g., Li-S) with improved safety considerations (e.g., non-flammable SSEs). The reviewer had no concerns about alignment with or relevance to DOE objectives for electrochemical energy storage.

Reviewer 2:
The reviewer replied that project tasks are well aligned with VTO goals, adding that SSEs are an enabler to a long cycle life in Li-metal batteries.

Reviewer 3:
The reviewer commented that development of safer, reliable, and flexible solid-state Li-metal batteries utilizing hybrid SSE exhibiting energy density 350 Wh/kg and cycle life of approximately 1,000 cycles will meet the DOE objectives.

Reviewer 4:
The reviewer said a flexible solid-state electrolyte coupled with a Li-sulfur cell chemistry can enable higher energy density, which helps with lowering cell cost with respect to dollars per kilowatt-hour.

Reviewer 5:
The reviewer described this project's support of overall DOE objectives as good.

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

Reviewer 1:
The reviewer indicated the current resources are sufficient to achieve the project goals.

Reviewer 2:
The reviewer said the resources are sufficient for the proposed tasking. The budget is reasonable.

Reviewer 3:
The reviewer replied the resources available to the project team seem to be sufficient to complete the project and report on the final milestone.

Reviewer 4:
The reviewer agreed the team has sufficient resources to meet the stated milestones with regard to both equipment and staff.

Reviewer 5:
The reviewer commented that project resources are okay.

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)

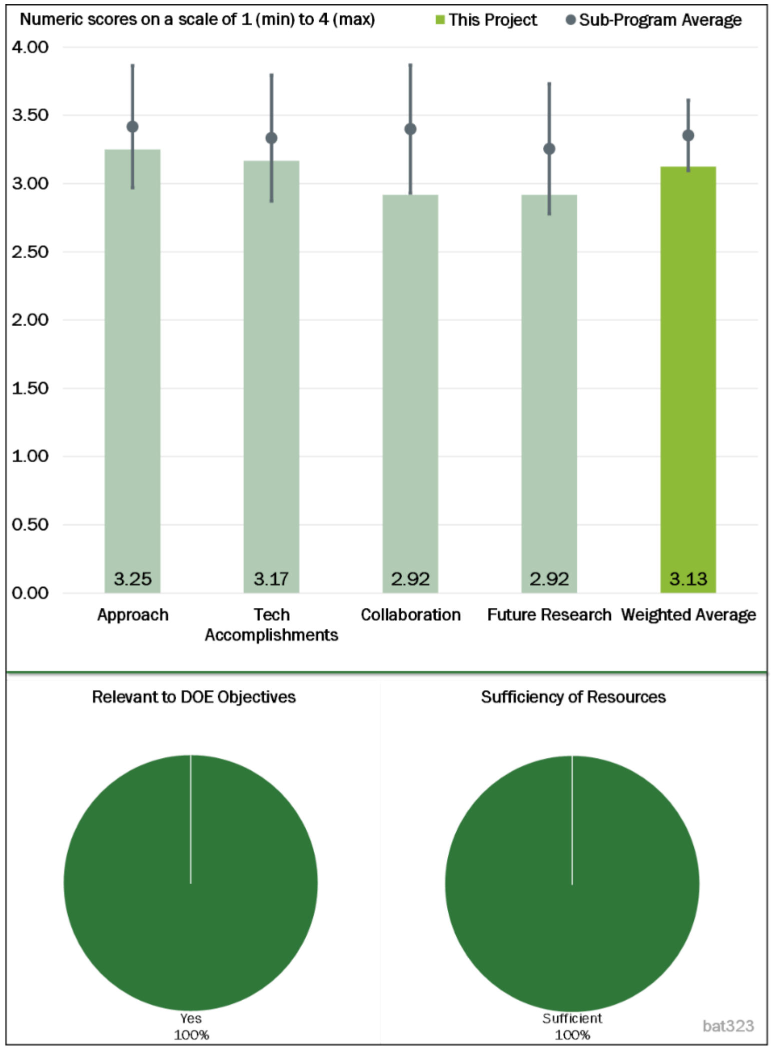

Figure 2-38 – Presentation Number: bat323 Presentation Title: Self-Forming Thin Interphases and Electrodes Enabling 3-D Structured High Energy Density Batteries Principal Investigator: Glenn Amatucci (Rutgers University)

Presenter
Glenn Amatucci, Rutgers University

Reviewer Sample Size
A total of 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 found the approach to be a very innovative, high-risk high-payoff one.

Reviewer 2:
The reviewer commented that the program is well designed to address most of the technical barriers. The reviewer noted that limitations of fluoride-ion transport and electron transport under static conditions may be high risk but also offer a high reward if these issues are addressed. Overall, the project is rationally designed.

Reviewer 3:
The reviewer stated that the approach to self-forming an interphase and electrode is quite novel and effective to address the low-energy-density, cost, and safety issues.

Reviewer 4:
The reviewer remarked that an in-situ formed, solid-state battery can inherently help the interface. Coupling the Li-metal anode and metal-fluoride cathode can lead to a high energy density.

Reviewer 5:
The reviewer wrote that the concept is appealing. However, the reviewer suggested that the PI should provide more details about the specific materials explored for implementing the concept.

Reviewer 6:
It was difficult for the reviewer to determine how close the program is to achieving the deliverables because it is not clear what size battery is being cycled. From the data presented, however, it appeared to the reviewer that the program is on track.

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:

Reviewer 2:
The reviewer said there are a lot of encouraging data, noting that energy density exceeds the target.

Reviewer 3:
The reviewer wrote that owing to the technical difficulties of this approach, the accomplishments and progress are noteworthy. The reviewer added the high-risk, high-reward nature of the project makes this approach worthwhile to explore.

Reviewer 4:
The reviewer stated that the key technical accomplishments of cell-design optimization have been properly achieved according to the project progress. The technical accomplishments made in the project are satisfactory.

Reviewer 5:
The reviewer indicated that the PI has demonstrated a 12V cell, adding that the cycling stability needs to be improved.

Reviewer 6:
The reviewer replied that the project met its milestones and go/no-go decision points. However, it was hard for the reviewer to evaluate exactly how the battery works as some details of the chemistry are not disclosed. The reviewer added that degradation at interfaces is not clear and needs to be examined.

Reviewer 7:
The reviewer remarked that the PI still does not provide much technical detail about the materials investigated, as well as data and graphs to support key accomplishments. The response to the last review that "The reviewer is correct and only limited information could be made public during the presentation" is unacceptable this time because the PI has had ample time to submit patent applications.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said there is no external collaboration but apparently the team is well coordinated based on the results.

Reviewer 2:
The reviewer noted it is a stand-alone project within the program without collaborations and does not help or influence other projects within the program.

Reviewer 3:
It was unclear to the reviewer whether the project has advanced sufficiently to need additional collaborators as the PI indicated in the response to the last review that "...we plan on bringing on other teams when the project is further along and we will require other expertise that we do not have on site."

Reviewer 4:
The reviewer wrote that the collaboration in the interdisciplinary team at Rutgers University is sufficient in the current early high-risk stage. When the project proceeds further, collaboration with other teams may be able to facilitate the progress.

Reviewer 5:
The reviewer suggested that more collaboration may be needed in the next step to verify the technology.

Reviewer 6:
The reviewer suggested more collaborations to better accomplish 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 wrote that the proposed research is reasonable with numerical targets.

Reviewer 2:
The reviewer stated that the proposed research is appropriate considering the low technical maturity of this project.

Reviewer 3:
The reviewer replied that the proposed future research on applying nano-layered electrode architecture is effectively planned and reasonable but has high risk.

Reviewer 4:
The reviewer wrote "no comment."

Reviewer 5:
The reviewer responded that the proposed plan is good because electronic and mechanical contact at interfaces is unclear, but it is very important for increasing rate and limiting capacity fade.

Reviewer 6:
The reviewer remarked that the proposed future research is vague, and that it also does not address important issues such as diffusion-induced stress, mechanical failures, and high-rate charging capabilities.

Reviewer 7:
The reviewer wrote "no comment."

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

Reviewer 1:
The reviewer indicated the project supports the DOE objectives well, as the proposed cell will show high voltage and energy density greater than 400 Wh/kg.

Reviewer 2:
The reviewer replied, yes, adding that energy density, cost, and safety of batteries are all DOE's primary objectives.

Reviewer 3:
The reviewer noted this is a high-risk, high-reward program that would not be funded by industry, so it is very appropriate for DOE objectives.

Reviewer 4:
The reviewer commented that, if successful, this project will lead to a cell with very high energy density.

Reviewer 5:
The reviewer said this project develops a novel manufacturing method of safe batteries.

Reviewer 6:
The concept may lead to high-energy-density batteries, but the reviewer added that the durability and high-rate capability are yet to be demonstrated.

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

Reviewer 1:
The reviewer described the project as well executed within the given resources.

Reviewer 2:
The reviewer said the resources for the project are adequate to achieve the milestones in a timely manner.

Reviewer 3:
The reviewer said the team seems to have all the resources necessary.

Reviewer 4:
The reviewer said the resources are sufficient.

Reviewer 5:
The reviewer commented that it is appropriately funded for low technical-maturity level as exploratory research.

Reviewer 6:
The reviewer wrote no comment.

Presentation Number: bat326
Presentation Title: Self-Assembling and Self-Healing Rechargeable Lithium Batteries
Principal Investigator: Yet Chiang-Ming (Massachusetts Institute of Technology)

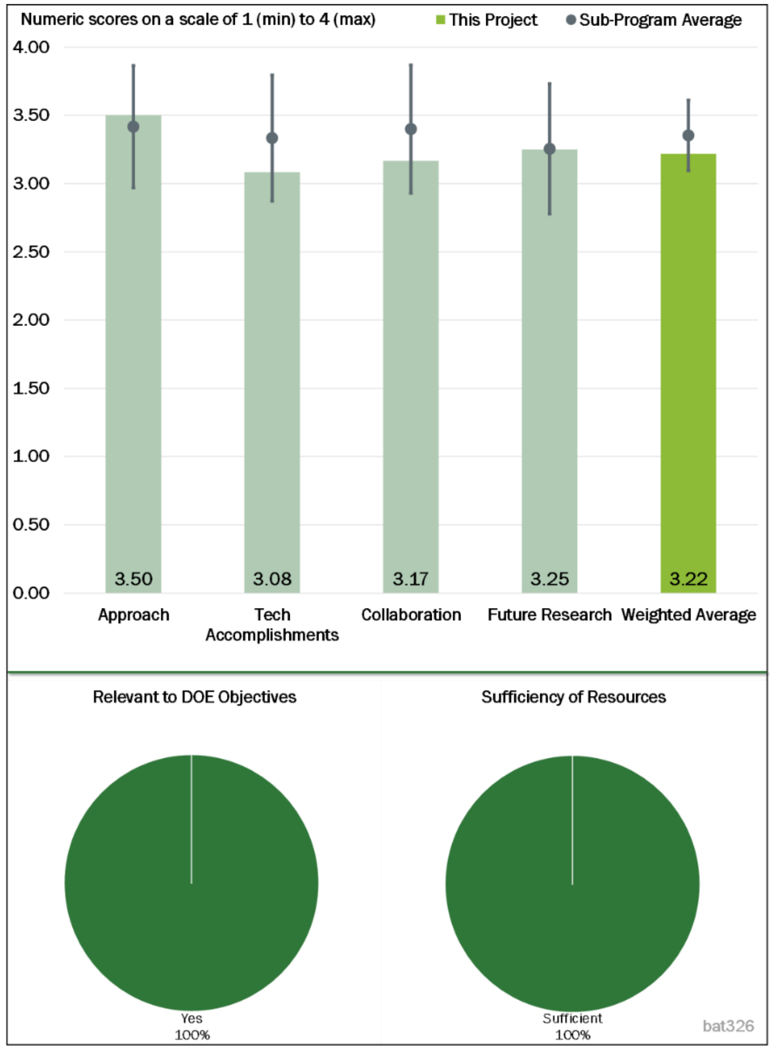

Figure 2-39 – Presentation Number: bat326 Presentation Title: Self-Assembling and Self-Healing Rechargeable Lithium Batteries Principal Investigator: Yet Chiang-Ming (Massachusetts Institute of Technology)

Presenter

Yet-Ming Chiang, Massachusetts Institute of Technology

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 described the approach as a novel and beautiful one.

Reviewer 2:

Overall, this is a well thought out research effort, the reviewer wrote, with a clear hypothesis, appropriate methods, and a clear description of the results and remaining gaps. The project is producing results that can help advance this field.

Reviewer 3:

The reviewer explained that the project used fluorine (F)-containing solvent as the source for the formation of LiF at the interface. The LiF-enriched SEI exhibits great performance. This project is well designed and feasible.

Reviewer 4:

The reviewer stated that leveraging the intrinsic reaction between Li and halides to self-form Li halide SSEs is an effective approach to mitigate Li dendrites.

Reviewer 5:

This work is aimed at simple Li metal anode technology based on fluoride containing SEI formation from fluorinated solvents such as FEC. If successful, the reviewer wrote, this approach work will address the battery cost barrier through the development of higher energy battery cells. The approach does not seem to require expensive materials or manufacturing processes. There is a good rationale for solvent selection and testing of self-assembling Li metal anodes.

Reviewer 6:

The reviewer indicated that there are two challenges in using Li-metal: the first is that it forms dendrites that eventually short the cell with repetitive cycling and the second is that the SEI does not completely stop the side reactions, which leads to loss of Li metal on every cycle until there is not enough Li to fully charge the cell. Many attempts by previous researchers have led to improvements in one but worsening of the other.

From a reading of their approach, it appeared to the reviewer that the project team is trying to solve problem one by developing halide-based SEIs that lead to compact Li deposition. However, the reviewer said they do not provide a CE target based on the amount of excess Li they are proposing that will allow them to get to 350 cycles and eventually to 1,000 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 loved the interplay between theory and experiment but the presenter could not answer a question about where the fade is coming from. This suggests that there is something very fundamental that is not being understood. The reviewer asked if this invalidates some of the work.

Reviewer 2:

The reviewer found that the results of the project are good, demonstrating improved cycling over a baseline. A challenge is that in order to get more than 250 cycles, an N:/P electrode ratio of 2.5 is needed, which means the Li is serving as a large reservoir, and also the electrolyte is in excess and is likely getting chewed up. So, the continued challenges of cycling Li in a liquid electrolyte are present. The reviewer noted that the PIs are well aware that barriers remain for this approach to work and state this clearly; this is very helpful and honest to have from the PIs themselves.

Reviewer 3:

The reviewer stated that a thin Li anode was used to evaluate the self-formed interface in both a Li-Li cell and Li- $LiCoO_2$ full cells. The cells show great performance, meeting the milestones.

Reviewer 4:

The reviewer explained that substantial cycle life has been demonstrated with self-assembled Li-metal electrodes in Li-Li asymmetric cell tests with fluorinated electrolytes, particularly FEC, in comparison to base solvents. These films have been characterized by XPS and SEM cross-sections. The reviewer elaborated that cross-sections show compact active layers of active material on the thin Li films. It was not clear to the reviewer how thick the active material layers are in comparison to the Li-metal reacted and it would be useful to estimate the porosity of the active material and track its thickness and composition throughout the cycle life. The reviewer suggested more characterization would be useful.

The reviewer stated that it is promising to see full-cell experiments included with up to 300 cycles shown. However, the details of these experiments are not clear. One set of experiments apparently utilizes an LCO cathode against a 20-µm Li electrode and the N:P ratio is listed as 1:1. The initial cell capacity is about 4 mAh/cm^2. However, the 20-µm Li electrode should have a capacity of about 8 mAh/cm^2. The reviewer asked whether the cathode capacity is 4 mAh/cm^2 or 8 mAh/cm^2. It seems either the N:P ratio is 2 or the testing is performed at 50% depth of discharge (DOD). In a second set of experiments, the N:P ratio is listed as 25 for a 50-µm Li film, which again seems inconsistent. It would also be useful to understand the degradation mode especially with the higher N:P ratio where the cell should be positive limited.

The reviewer indicated that electrolyte content was not provided in the presentation. However, in last year’s review, the electrolyte content seemed to be about 10 mAh/g, which is several times the amount recommended by Battery500 for realistic coin-cell, cycle-life measurements.

According to the reviewer, it would be useful to study the CE and cycle life as a function of DOD as it might shed light on the degradation mechanism of these novel Li-metal active materials.

Reviewer 5:
The reviewer noted that the performer demonstrated good cycle life that was attributed to the decomposition of fluoride (F^-) to self-form LiF, just like iodide (I^-) in solution to form lithium iodine (LiI). LiF-rich SEI is key to their self-formed interface. It is unclear if the thin LiF-rich SEI will be sufficient to mitigate Li dendrites. They needed to show how they projected 350 Wh/kg (assume packaged?) at 3 mAh/cm^2 loading, and 50-µm Li with N:P ratio of 2.5.

Reviewer 6:
The reviewer pointed out that the researchers' goal is to define some descriptors that can be used to design new Li-halide based SEIs. Up to now, it appears they have tested a number of solvents and measured their descriptors and effect on CE, but the reviewer did not see where they have developed a quantitative model based on the descriptors that would explain their results.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said a true collaboration appears present.

Reviewer 2:
The reviewer replied that the key collaboration partner is listed.

Reviewer 3:
The reviewer stated that the industrial partner is good.

Reviewer 4:
This appears to be a stand-alone project, and the reviewer was unaware of a team of researchers organized to work together on this problem. The project team does share its results with a battery company, 24M, which tests the team's materials in cells for independent verification.

Reviewer 5:
The reviewer noted that the performer has identified 24M as the transition partner for their technologies.

Reviewer 6:
The reviewer suggested more partners be included on 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 remarked that there is a very bright future for this idea.

Reviewer 2:
The reviewer found the proposed research reasonable.

Reviewer 3:
The reviewer noted the project is coming to a close and added that more details on future work would be helpful, but are likely not included because the project is ending.

Reviewer 4:
The reviewer explained that the proposed future work is to identify new substances to try, based on their modeling efforts; test the materials in cells; and test the effect of pressure. The reviewer would like to have seen how well the model is doing in predicting CE. The last two are very empirical. It appeared to the reviewer that depending on the solvent and additives used, one gets a different density of Li plating. They say that LiF-rich SEIs promote densification of the Li, but the PIs also show that 1-(trifluoromethyl)ethylene carbonate (CF_3-EC) has the most LiF in the SEI from XPS data but it has the worst coulombic efficiency. The reviewer was unsure how the project team will resolve this.

Reviewer 5:
The reviewer pointed out that there is not much time left in this project, which ends in December 2019. The expressed interest in stack pressure seem reasonable. The reviewer recommended more emphasis on consistent experiments with well-defined and well-controlled electrode capacities, N:P ratios, DOD, and reasonable electrolyte content capable of achieving the 350 Wh/kg target in a convincing manner.

Reviewer 6:
The reviewer said that to mitigate Li dendrites, the project team needed to demonstrate self-healing with their fluorinated solvents.

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

Reviewer 1:
The reviewer described a novel approach to get to higher energy cells.

Reviewer 2:
The reviewer said it is clearly focused and making contributions to Li-metal anodes.

Reviewer 3:
The reviewer stated that trying to understand how to reduce CE on Li is critical to the success of this anode.

Reviewer 4:
A self-formed, self-healed (SSE is key to mitigating Li dendrites in a rechargeable Li-metal cell.

Reviewer 5:
The reviewer explained that self-forming, self-healing interfaces between the Li metal and the electrolyte is simple and scalable and enables very high energy density batteries.

Reviewer 6:
The reviewer noted this is challenging, high-risk R&D aimed at breakthrough Li-metal electrode technology that could enable higher energy density battery cells with lower cost. The reviewer added that relevance to fast-charging objectives is probably premature.

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

Reviewer 1:
The reviewer stated that the project team has sufficient resources to demonstrate the feasibility of a self-formed, self-healed SSE.

Reviewer 2:
The reviewer wrote that the resources appear appropriate for the work completed.

Reviewer 3:
The reviewer replied that there are sufficient funds for this trial experiment.

Reviewer 4:
The reviewer said no evidence of resource limitations was provided.

Reviewer 5:
The reviewer wrote that the resources are sufficient.

Reviewer 6:
Resources were described by this reviewer as okay.

Presentation Number: bat327
Presentation Title: Engineering Approaches to Dendrite-Free Lithium Anodes
Principal Investigator: Prashant Kumta (University of Pittsburgh)

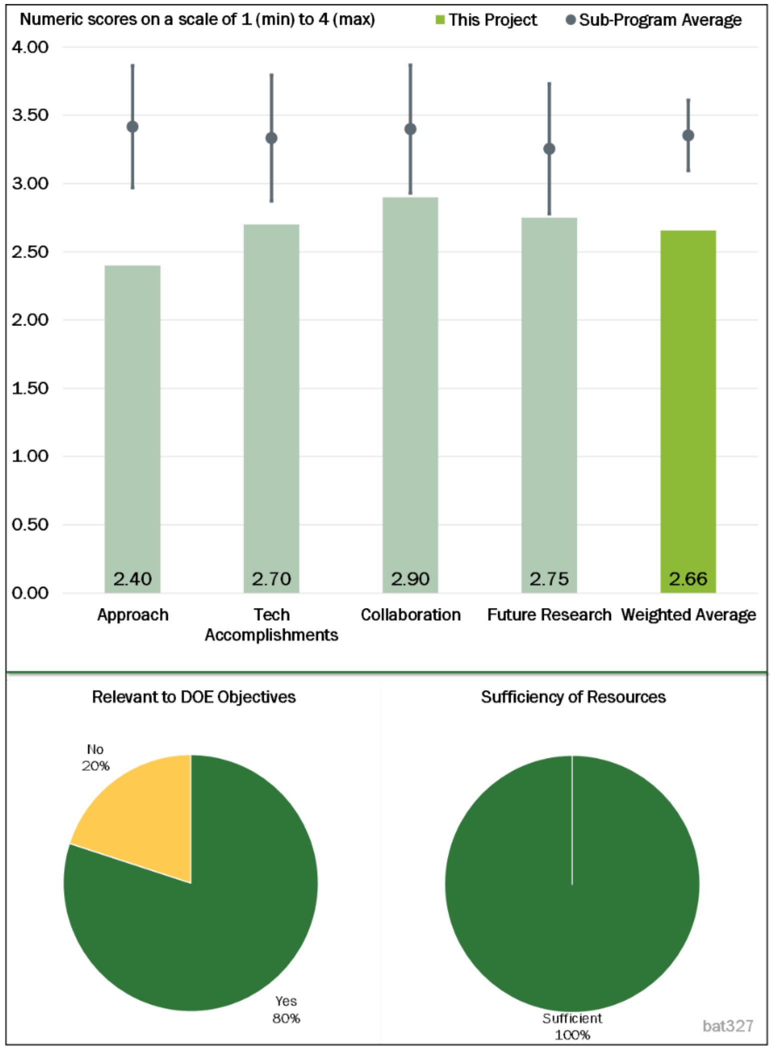

Figure 2-40 – Presentation Number: bat327 Presentation Title: Engineering Approaches to Dendrite-Free Lithium Anodes Principal Investigator: Prashant Kumta (University of Pittsburgh)

Presenter

Prashant Kumta, University of Pittsburgh

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 project is well designed and feasible, the reviewer wrote, and added that the PI is mainly focusing on the interface between deposited Li and current collectors. The reviewer suggested it would be good to study the effect of the interface between the electrolyte and deposited Li as well.

Reviewer 2:

The reviewer commented that the work is aimed at materials engineering design of substrates to eliminate dendrite formation at Li-metal anodes with increased energy density. The reviewer suggested it would presumably overcome limited cycle life and achieve lower cost through increased energy density. The reviewer noted that multiple approaches to engineering design of substrates are being pursued.

Reviewer 3:

The reviewer observed that the project team proposed multiple approaches to overcome Li dendrite and mossy Li formation on the surface of Cu, including multicomponent alloys (MCAs), structurally isomorphous alloys (SIAs), and surface coatings. The reviewer commented that these approaches are, at best, useful to affecting Li nucleation at the Cu-current collector, but not the growth processes of Li dendrites and mossy Li by electroplating and stripping since the electrolyte has a major effect.

The reviewer suggested that the project team seemed to be confused about “interfacial energy” and “enthalpy” of formation of alloys, as pointed out by one of the reviewers during the AMR meeting (Slide 8. More importantly, there is no clear correlation between interfacial energy, which controls nucleation, and the enthalpy of formation, which affects the formation of bulk phases.

Reviewer 4:
The reviewer said the slide on Approaches was so wordy that it was unclear what the main thrusts of the work was. The approaches seemed to focus on understanding the impact of current collector on Li dendrites. The reviewer commented that the project team needed to explain the impact (the "so what") of its approaches without relying too much on modeling equations.

Reviewer 5:
The reviewer remarked that it was very hard to follow this presentation. It sounded to the reviewer like the idea is to modify the current collector, but it was hard to understand how this will impact plating, when the current collector is covered by Li-metal, and we are looking at Li plating on Li (with lots of SEI around), not Li plating on the current collector. The reviewer also had serious concerns that the Li-Li cell results are for cells that have soft shorted. This can be overlooked and result in excellent cycling, but of electrons, not Li.

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 indicated the PI has developed a few SIA electrodes that exhibit high CE and cycle life at large current.

Reviewer 2:
The reviewer noted that a significant achievement was 300 cycles at 4 mAh/cm^2 with MCAs showing good progress to the go/no-go target of 1,000 cycles. Other approaches appear not to be so successful. The reviewer recommended that cycle life under partial depth-of-discharge conditions, where a fresh surface is not provided prior to each charge, also be measured. Dendritic growth can be stimulated by partial depth-of-discharge conditions, which would also represent the usual real-world application situation. The reviewer also noted that no status was given of progress for the last two milestones due July and September 2019 and that no discussion of cost status or plan to study Li-S or other full-cell was provided.

Reviewer 3:
In spite of their modified Gibbs Thomson modeling, it was unclear to the reviewer how the adhesion between Li metal and current collector impact the Li dendrites. The reported good cycling data for MCA and ISA alloy current collectors were based on thick 100- µm Li metal and low loading of 0.5 mAh/cm^2, which might not be relevant for a practical full cell.

Reviewer 4:
The reviewer concluded that there is insufficient information, such as the composition and structure of the MCAs and SIAs, presented for this reviewer to effectively evaluate the technical accomplishments. The reviewer found this puzzling since there is a long list of publications that are either "under preparation" or "under review." The PI should have, therefore, presented some details about the materials systems.

The reviewer also noted that the equation to calculate "interfacial energy" (Slide 12 is incorrect since interfacial energy must take into account the segregation of elements at the interface, which are not necessarily the same as bulk composition. Also, the equation neglected the heats of mixing terms.

Reviewer 5:
From the presentation, the reviewer stated it was difficult to understand exactly what has been accomplished. The reviewer looked at the presentation slides, and it looks like there are no published papers from this project to date. The reviewer concluded that the basic hypothesis is not clear, and the significance of the cell testing is a question in the reviewer's mind.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said the P.I. identified a transition partner for their technology and provided clear descriptions of the roles of each partner.

Reviewer 2:
The reviewer noted that collaboration with key partners is listed.

Reviewer 3:
The reviewer suggested that the project team should send samples for independent evaluations by others in the R&D community.

Reviewer 4:
The reviewer remarked that the project team needs to strengthen its collaborations.

Reviewer 5:
The reviewer commented that there appears to be some collaboration, although the extent is hard to follow.

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 the proposed future research reasonable with clear numerical milestones to achieve the objectives of the project.

Reviewer 2:
The reviewer noted the project is due to end in September 2019.

Reviewer 3:
The reviewer commented that the project team needed to demonstrate performance in a full cell using their alloy current collectors and compare the CE with that of a typical current collector, using practical loadings of greater than 2-3 mAh/cm^2, an N:P electrode ratio of approximately 1.0, and a thin Li-metal foil of less than 20-µm.

Reviewer 4:
A list of metrics is given, the reviewer wrote, but it was hard to tell what will be done to achieve those metrics.

Reviewer 5:
Because the materials systems are undisclosed, this reviewer could not evaluate the likelihood of the project team making further improvements to reach the various targets listed under the "Proposed Future Work."

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

Reviewer 1:
The reviewer project stated that the project is focused on the DOE goals and hopefully something can be learned from the results.

Reviewer 2:
If successful, the reviewer wrote, the project will help enable Li-metal electrodes in practical applications.

Reviewer 3:
The reviewer replied that this project is aimed at development of Li-metal anode batteries supporting overall DOE objectives of higher energy density batteries with lower cost.

Reviewer 4:
The reviewer stated that suppressing dendrite formation is the long-term goal of achieving high energy Limetal anodes.

Reviewer 5:
It was not clear to the reviewer from the presentation if an engineered electrode can mitigate Li dendrites.

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 performer has sufficient resources to demonstrate an engineered electrode that can mitigate Li dendrites.

Reviewer 2:
The reviewer found the resources are reasonable and sufficient.

Reviewer 3:
The reviewer replied the team seems to have sufficient resources.

Reviewer 4:
The reviewer indicated the resources appear sufficient.

Reviewer 5:
The reviewer said there was no evidence of insufficient resources.

Presentation Number: bat328
Presentation Title: Dendrite-Growth Morphology Modeling in Liquid and Solid Electrolytes
Principal Investigator: Yue Qi (Michigan State University)

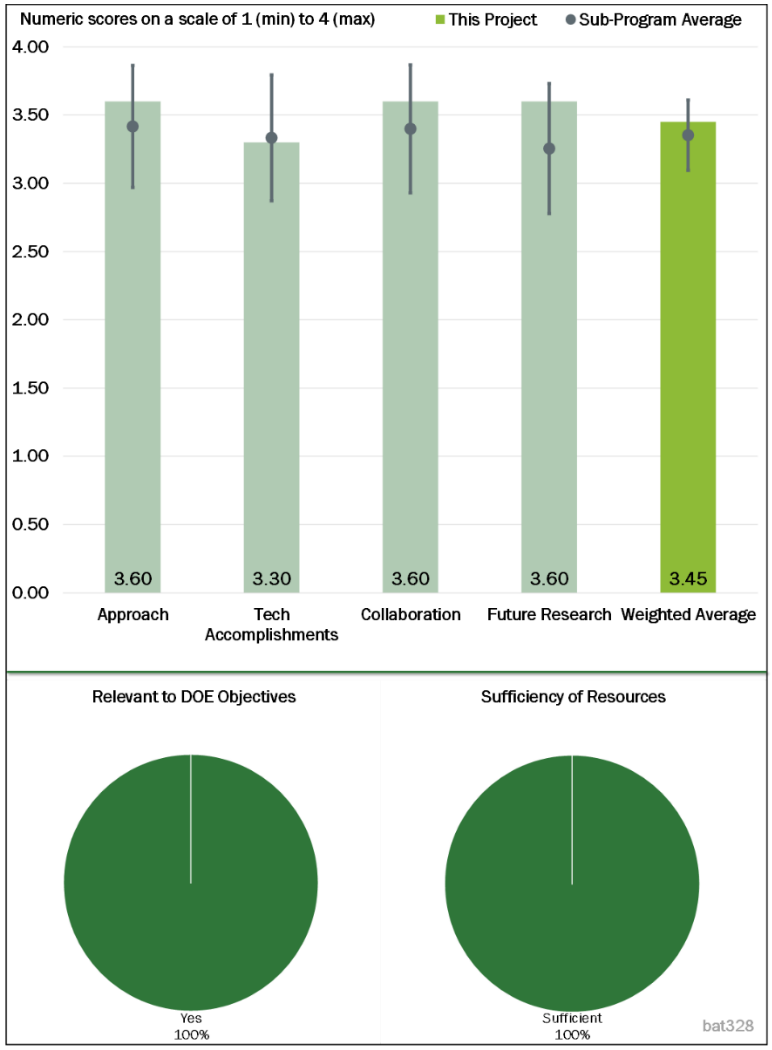

Figure 2-41 – Presentation Number: bat328 Presentation Title: Dendrite-Growth Morphology Modeling in Liquid and Solid Electrolytes Principal Investigator: Yue Qi (Michigan State University)

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 stated that the project is well designed and feasible, adding that there is a good mix of calculation and validating experiments. Some important results were obtained and reported such as a better understanding of potential reasons for dendrite formation.

Reviewer 2:

While the majority of the modeling projects focus on understanding perfect materials, the reviewer noted that dendrite growth is known to preferentially occur in non-perfect materials. This project aims to comprehensively address dendrite growth in grain boundaries and through defects that introduce states inside of the band gap making SEI or solid electrolyte less electronically insulating. The reviewer concluded it is a timely and well-planned project combining atomistic and mesoscale modeling, adding that there is a good connection with experiments performed by other groups.

Reviewer 3:

According to the reviewer, the overall goal was to understand and predict Li-dendrite formation in liquid and solid-state electrolytes. The hopes were with this understanding to perhaps create artificial SEI layers to prevent or mitigate Li-dendrite formation. Initial results set the project team to focus on further studying LLZO over other solid-state electrolytes. The reviewer observed that the project team initially saw that LLZO has localized electrons trapped on the surface, whereas lithium phosphorus oxynitride (LiPON) and other solid electrolytes do not. The project team then set out to understand how this surface difference results in SEI formation at these surfaces within grain boundaries of polycrystalline LLZO. The reviewer commented that the project team has found, through modeling results, that the trapped electrons at the surface of the LLZO accelerate Li-dendrite growth. The project team has able to compare their results with that of liquid electrolytes. Additionally, the reviewer remarked, when looking at the surfaces the project team has found that LiS passivation layers are better than Li_2O passivation.

Overall, the reviewer remarked that the work has been well executed. However, one challenge is translating modeling results to real cell performance. For example, the reviewer asked how a native carbonate on the surface of the LLZO changes the predictions of the project team, which needs to show more experimental work to back up predictions.

Reviewer 4:

The reviewer explained that the highlight of the computational approach is an integrated framework, which includes an atomistically informed (DFT calculations) phase-field model to study the electrochemical and mechanics-coupled physical processes responsible for Li-dendrite morphology evolution for liquid and solid electrolytes. The fundamental physics from the atomistic calculations is certainly a key driver in this approach, according to the reviewer.

Reviewer 5:

The reviewer described the proposed multi-scale, multi-physics model as addressing the problem of dendrite formation and growth. The evolution of the Li dendrite is a complex phenomenon that depends on several conditions such as electrochemical reactions and mechanical properties of the solid electrolyte; for that reason, a model able to have in consideration both properties will provide new insights about dendrite formation and growth. The reviewer found the procedure to be well designed, starting from atomistic simulations to calculate some properties of possible solid-electrolyte materials. Simultaneously, experimental results validate the calculations done in the atomistic simulations. The reviewer noted that parameters to develop the multi-scale, multi-physics model are taken from the atomistic simulations and experimental calculations. The reviewer elaborated that even though the environment of a dendrite growth in a liquid electrolyte and a solid electrolyte are different, some procedures can be transferred from one to the other, such as the electron-trapping mechanism in which the project team proved that the calculation done for solid electrolyte can be also used for the SEI formed when the Li metal is in contact with a liquid electrolyte.

The reviewer stated that experimental calculations to analyze the morphology of the dendrite formation are performed, but it was not well stablished how those experiments are linked with the model development.

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 that the team has made substantial progress to achieve the program objectives.

Reviewer 2:

The reviewer explained that a combination of DFT, reactive force field, and mesoscale phase-field simulations revealed the influence of defects, grain boundaries, and mechano-chemical response (Li_2O shrinkage and crack formation) on the initial stages of the Li-metal dendrite growth. The mechanism behind the experimentally stabilized SEI on the Li metal was suggested based upon modeling. The reviewer applauded the excellent dissemination of the results in eight published manuscripts in high-impact journals and three submitted manuscripts.

The reviewer was quite impressed with the broad scope of modeling techniques that were applied to investigate critical properties of solid electrolytes and SEI.

Reviewer 3:

The reviewer stated that among the multi-faceted, physics-based advancements made in this project, an important highlight is the excess electro-trapping mechanism for solid electrolytes (such as LLZO) and how it affects dendrite growth. This allows for further adoption of this strategy for stabilizing the SEI for liquid electrolytes with Li-metal anodes, according to the reviewer.

Reviewer 4:

The reviewer found that there is a strong improvement with respect to last year. So far, the project team showed a working multi-scale, multi-physics model of dendrite growth of a polycrystalline LLZO based on atomistic simulations and experimental calculations. The model can predict capacity fading and isolated nucleation; however, the reviewer went on to say that comparison with experimental results is needed in order to validate the model. Studies of specific phenomena in dendrite formation and growth have been performed but there is not a clear path in which all these studies will converge to develop the multi-scale, multi-physics model. The reviewer indicated that battery operating conditions, such as rest time and charge and discharge, have not been addressed in the proposed model.

Reviewer 5:

The reviewer indicated the project team has built a good model for showing grain boundary SEI and Li-dendrite growth. The project team has additionally shown that Li_2O and LiS as passivation layers perform differently. However, the reviewer commented that more experimental work to back up these hypotheses is needed.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer wrote that the PIs have shown an excellent coordination between the atomistic and mesoscale (continuum) levels and initiated collaborations with experimental teams providing meaningful feedback on the mechanisms of dendrite growth and avenues to prevent it.

Reviewer 2:

The reviewer found synergistic and productive collaboration with experimental (synthesis, diagnostics, and characterization) counterparts (e.g., SNL, PNNL, the University of Arkansas, the University of Maryland, and the University of Houston) that is noteworthy.

Reviewer 3:

The reviewer said the program seems to be well coordinated.

Reviewer 4:

The reviewer remarked that several calculations and experiments have to be performed in order to develop a multi-scale, multi-physics model. The collaboration is well established with several institutions running particular simulations and experiments, addressing several phenomena occurring in a solid-state battery with a Li-metal anode such as Li electrodeposition, possible additives to develop a better SEI, morphology of Li in contact with the electrolyte, and possible SEI coating. The reviewer noted that all these calculations and experiments will provide new data in order to develop the multi-scale, multi-physics model.

Reviewer 5:

The reviewer said the project team has shown good collaborative effort in their work as represented by their publication record. However, the reviewer suggested that there still needs to be more work on developing better experimental results.

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

Reviewer 1:
The reviewer concluded the proposed future research clearly identifies exploring the role and potential for coating layers for solid electrolytes, and also studying the SEI structure interaction with dendrite growth.

Reviewer 2:
The reviewer wrote the future work is appropriate and feasible.

Reviewer 3:
The reviewer explained that Li-dendrite formation and growth is a complex phenomenon that occurs in Li batteries. In order to develop a full model with the ability to simultaneously predict mechanical, electrical, and chemical properties, several atomistic simulations in conjunction with experiments have to be performed; however, the project team has already developed a model of Li-dendrite formation and growth in contact with a solid electrolyte (LLZO) combining atomistic simulations and experiments results, capable of predicting capacity fading and isolated nucleation, showing their experience and ability to address some of the issues involved in Li dendrite growth. The reviewer concluded that proposed future research for the project team +follows the line to go further in the development of a more accurate model, combining experimental and computational calculations, including the addition of a coating layer between the Li and the electrolyte.

Reviewer 4:
The reviewer said the project sharply focuses on the critical barriers. The reviewer fully agrees with the focus on the proposed work, which is quite ambitious (might be too ambitious). If planned research that is focused on establishing a relationship between the Li-SEI interface, roughness, adhesion, dendrite morphology and multicomponent SEI layers is, indeed, successful, the impact of the project is expected to be significant.

Reviewer 5:
The reviewer stated that team’s proposed work on further understanding the SEI structure, predicting electron transport at the grain boundaries, and dopant-dependent grain boundary electron trapping are good theoretical work that can help in understanding the Li dendrite formation and the results could help in the design of new passivation chemistries. However, the reviewer added that more future work is needed to correlate their predictions with experimental work.

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

Reviewer 1:
The reviewer found that the project is aligned with the goal to advance the Li-metal-based battery technology in improving cycling efficiency and life.

Reviewer 2:
The reviewer agreed that all the effort follows the guidelines and vision provided by DOE’s VTO.

Reviewer 3:
The reviewer explained that the program has developed knowledge that can be useful to understand and enable the use of Li metal in both solid- and liquid-electrolyte systems. This could lead to a much higher energy density and consequently a lower cost per kilowatt-hour, which is a driving goal of the DOE to increase adoption of EVs and hybrid electric vehicles (HEVs).

Reviewer 4:
The reviewer indicated that stabilization of the Li-metal via rational SEI or solid-electrolyte design is important for increasing Li battery energy density and decreasing cost.

Reviewer 5:
The reviewer noted that this work on fundamentally understanding the grain boundaries, SEI formation, and preventing Li dendrites is important for further advancing SSEs and is needed if liquid electrolytes are going to be replaced. The reviewer added, however, the project team needs more work on relevant testing protocols to support their work.

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

Reviewer 1:
According to the reviewer, excellent planning and resource utilization made this project successful.

Reviewer 2:
The reviewer said the project team has shown it has the ability to build models to predict the surface SEI and have shown experimentally that passivations matter.

Reviewer 3:
The reviewer remarked that the project team is well placed for required computational and collaborative experimental resources for the success of this project.

Reviewer 4:
The reviewer found appropriate funding level for the objectives.

Reviewer 5:
The reviewer stated that everything seems to indicate that the project team has enough resources.

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)

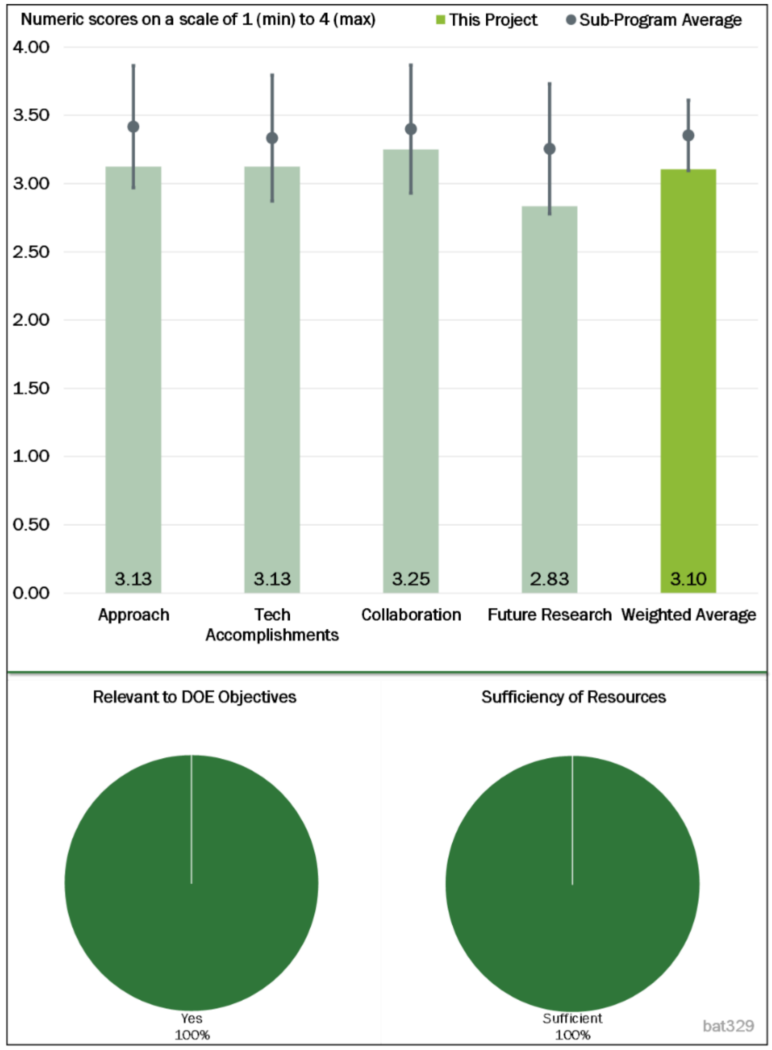

Figure 2-42 – Presentation Number: bat329 Presentation Title: Understanding and Strategies for Controlled Interfacial Phenomena in Lithium-Ion Batteries and Beyond Principal Investigator: Perla Balbuena (Texas A&M University)

Presenter

Perla Balbuena, Texas A&M University

Reviewer Sample Size

A total of 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 there was a very nice integrated approach of multiple theoretical approaches coupled with experimental input and validation.

Reviewer 2:

The approach is good, the reviewer said, but makes some approximations such as the potentials used in MD simulations that could limit the reliability of the results. In addition, the modeling of nucleation is quite approximate and may limit the reliability of the results. The reviewer noted that the DFT calculations of surface reactions can provide useful information, but may also need to have a better account of the surrounding electrolyte and potential effect of defects.

Reviewer 3:

The reviewer explained that the objective was to evaluate and characterize the interfacial phenomena in Li- and silicon-metal anodes and how SEI products affect the electrodeposition of Li. The PIs have said they compared experiments to their modeling. The reviewer stated that the project team claims to have done experimental work; however, nothing was actually presented. Additionally, this project is 80% completed, but no work on Si-anode surface was presented. The reviewer said that more experimental work is needed to help guide the modeling to be more effective.

Reviewer 4:

The reviewer commented that most of the calculations do not lend themselves to experimental confirmation.

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 particularly appreciated the study of impurity effects on Li deposition and the study on solvent type on the Li-deposition process.

Reviewer 2:

The reviewer said accomplishments are good but are not connected to experiments.

Reviewer 3:

The reviewer remarked that what the project team has shown is their work on trying to understand how the charge-transfer phenomena change on different Li-surface passivation layers. They compared Li_2O, lithium carbonate (Li_2CO_3), and lithium hydroxide (LiOH). Their modeling shows that Li_2O holds a charge but is also still able to transfer electrons to the surface. They also show through modeling that the LiOH stores a charge, but less than Li_2O and that the OH^- groups tend to accumulate a charge. Lastly, Li_2CO_3 stores a charge but continuously exchanges charge with Li. The reviewer found this work to be interesting, but it would be really good to get modeling results to show how this is validated through experiments. It was hard for the reviewer to believe that this is relevant without those experiments. The project team also calculated the thermodynamic and kinetic properties of electrodeposition, which show that in the absence of an electric field, Li deposition is endothermic and, as the electric field is increased, it becomes exothermic. The reviewer asked if the project team could use analytical characterization techniques to validate this work. For example, the reviewer wanted to know if the project team could do an in-situ calorimetry study to confirm these results. Lastly, the reviewer stated that the project team claims to have looked at the silicon-anode surface. This was not presented in this review so it was unclear to the reviewer if the project team has already done this work.

Reviewer 4:

The reviewer stated that the computational studies have provided insight into various aspects of Li-anode interfaces of Li-ion batteries including the solid electrolyte interphase chemistry and reactivity and the effect of applied potential on Li deposition. Dendrite nucleation and growth were analyzed at nano and mesoscopic levels. Within the approximations used in the modeling approach, the reviewer mentioned that this work has provided explanations that should be helpful in designing improved battery materials for interfaces.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer described excellent collaboration with the project team in terms of complimentary capabilities.

Reviewer 2:

The reviewer found very good interaction with experimental groups such as Murugesan at PNNL.

Reviewer 3:

It was unclear to the reviewer how the project team used their experimental collaborators within this project, at least during the presentation. They have clearly and effectively used their modeling collaborators.

Reviewer 4:

Describing the collaboration as “Okay,” the reviewer said it would be nice to have known who did what.

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 researchers have a good plan for the last year of this project.

Reviewer 2:
The reviewer explained that the team would like to determine more accurately the SEI on Li-metal anodes. They want to apply artificial intelligence methods to cover a wider range of situations and develop alternative strategies for Li-metal anodes. The reviewer found that in their future work, there still is no indication that the project team will investigate the silicon surface and no indication that they are going to compare more experimental results to their computational work. The reviewer concluded that more collaboration is needed to validate the theory.

Reviewer 3:
The reviewer wrote that directions are good, but there are no indications of what new barriers will need to be overcome.

Reviewer 4:
The reviewer observed that the project is ending this year.

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

Reviewer 1:
The reviewer suggested that the work being carried out in this project is very relevant to the DOE mission for EVs and energy conservation.

Reviewer 2:
The reviewer said it was appropriate and very relevant to investigate interfacial phenomena in Li-metal and Si-alloy anodes. The interface with the electrolyte appears to be where all issues arise. The focus on Li metal is good, but the reviewer would like to have seen more first-principles' insight into the Si-SEI and why it is so different from the graphite SEI.

Reviewer 3:
The reviewer would like to have seen more connection to experiments. The reviewer pointed out that prediction of LiF and Li_2CO_3 is not a strong corroboration of the modeling.

Reviewer 4:
The reviewer stated that the project has the potential to be relevant to the overall DOE objectives, but that it was just unclear how the current work presented can be translated to experimental work.

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 there are appropriate resources.

Reviewer 2:
The reviewer replied the resources are sufficient.

Reviewer 3:

The reviewer indicated that it seems there are adequate resources; however, perhaps more experimental resources are needed to help link the theory with experiments.

Reviewer 4:

The reviewer wrote “Okay.”

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.

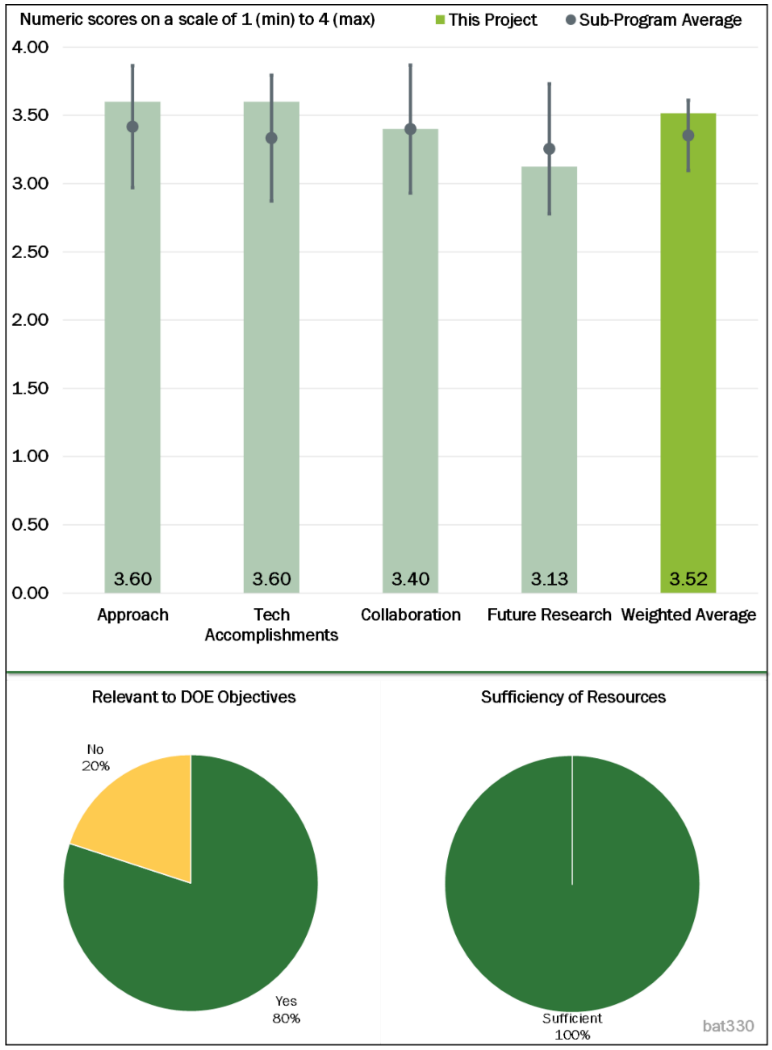

Figure 2-43 – Presentation Number: bat330 Presentation Title: Electrochemically Responsive, Self-Formed, Lithium-Ion Conductors for High-Performance Lithium-Metal Anodes Principal Investigator: Donghai Wang (Penn State University)

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:

Explaining that dendrite-free electrochemical Li-metal deposition is an extremely difficult problem and stable and high-capacity sulfur-electrode cycling is also an extremely challenging topic, the reviewer said both topics are also extremely important for future high energy storage systems. The reviewer found this project addresses both critical problems.

The reviewer elaborated that the project team has proposed and developed novel techniques to prevent Li-dendrite growth. In particular, the high-zeta potential, porous sponge approach is very novel, and results are very encouraging. The additive approach to improve S electrode stability is a viable approach. According to the reviewer, the project team focuses on very high loading S electrode (over 10 mg/cm^2). This is important to achieve high energy density.

Reviewer 2:

The reviewer commented that the effort is supporting DOE objectives by addressing a key challenge to the development of a Li-metal battery dendrites. The approach focuses on developing self-formed hybrid Li-ion conductors as a protective layer on the Li and a Li-ion affinity sponge anode that will increase local Li ion concentration and reduce concentration polarization. If successful, the reviewer wrote, these efforts would significantly lower battery cost by increasing cycle life.

Reviewer 3:

The reviewer said that overall this appears to be well organized work with appropriate methods and approaches. Various materials approaches are used to improve cycling with Li metal and S.

Reviewer 4:
The reviewer replied that the approach of using a Li-ion affinity sponge host to minimize the concentration gradient at the Li-metal and electrolyte interface, which helps to prevent dendrite growth of Li metal, is very novel and innovative. In addition, self-formed Li ion-conducting protective layers on Li-metal to prevent dendrite growth as well as minimizing SEI formation are also very innovative approaches. The reviewer added that the experimental work is well designed and feasible to address the major issues of Li-metal batteries such as dendrite formation and low CE. The PIs also address the major issue of S cathode such as high-S loading, S utilization, PS dissolution, and shuttling.

Reviewer 5:
This is a novel approach that the reviewer had not previously seen, but it does not deal with volumetric energy density.

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:
Finding that significant progress was achieved this year, the reviewer explained that the team showed that electro-kinetic surface conduction and electro-osmosis within a polyethylenimine sponge changes the Li-ion concentration and enables dendrite-free plating and stripping of Li with a high CE. In addition, organo-lithium sulfide (LixSy) and organo-lithium-phospho-sulfide (LixPySz) composite Li protection layers effectively suppress growth of dendritic Li.

Reviewer 2:
The reviewer remarked that significant progress has been made on the fundamental understanding of the concentration gradient effect at the Li-metal and electrolyte interface on the dendrite growth kinetics. It will be a great achievement if the PIs are able to determine the minimum concentration gradient that needs to be maintained at the Li-metal and electrolyte interface to prevent dendrite formation. The reviewer explained that a significant improvement of cycle life has been achieved using 3-D cross-linked porous polyethylenimine sponge (PPS), however, CE still needs to be improved for commercial realization. However, the reviewer said that a significant improvement of CE is achieved using Li-ion containing, hybrid Li-metal protection layer. Significant progress has been made on a high S-loaded cathode using a conventional electrolyte with additive showing higher S utilization and higher energy density in comparison to conventional electrolytes without additives. The reviewer further elaborated that the PIs also demonstrated the feasibility to achieve energy density of 350 Wh/kg for a Li-S cell using the developed Li-metal host anode and high S-loaded cathode utilizing an N:P electrode ratio of 1.5 and an E:S ratio of 5.

Reviewer 3:
The reviewer stated that the PI's team made significant progresses in both Li-metal deposition and a S electrode. The reviewer provided the following explanations for the Li-metal project:

The project team developed two new approaches to stabilize Li-metal electrochemical deposition. First, the project team used a high-zeta potential and highly porous sponge to contain Li deposition in the porous structure. The experimental results show the deposited Li-metal is confined in the porous sponge but does not form dendrites. The reviewer noted that the Li-metal stable-cycling performance is extended to over 400 cycles. The cells made with this confined Li-metal electrode and a LFP electrode cycle very well at limited N:P ratios. Secondly, the team developed an organo-sulfide stabilization layer for Li-metal surface protection. The cycling results are also very much improved compared to the baseline.

Regarding the sulfur-electrode project, the reviewer commented that the project team developed functional C-S-polymer composite cathodes that were fabricated with high S mass-loading ranging between 7 and 12 S/cm^2. The composite electrode has a capability of PS adsorption. The project team has also developed and used an electrolyte additive. The reviewer indicated that the project team has demonstrated a very high S loading electrode at 11 mg/cm^2 S at 1,200 mAh/g S utilization. This is a significant improvement from the baseline of 700 mAh/g.

Overall the team has made significant progresses in both the Li and the S projects.

Reviewer 4:
The reviewer found impressive results for a moderate E:S ratio of 5.

Reviewer 5:
The reviewer said the results are impressive for some evaluation criteria, but the CE is still too low (at least 99.95% is needed), and for the Li-S cells, the E:S ratio is still too high to make cells with overall compelling performance. Improvements in the N:P ratio are good, but the ratio of 1.5 is probably still too high.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found excellent collaboration exists between the Penn State team and PNNL.

Reviewer 2:
The reviewer replied that the PI has good collaborations with Pennsylvania State University (PSU) colleagues for theory as well as with PNNL for fabrication of Li-S full batteries.

Reviewer 3:
The reviewer said it appears that there is some good collaboration among team members.

Reviewer 4:
The reviewer remarked that this is mostly a single PI investigation project, although the PI also reach out to other groups within his own university with complimentary skills and PNNL to collaborate.

Reviewer 5:
The reviewer stated that the collaboration is only adequate, but maybe they do not need any additional partners

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

Reviewer 1:
The reviewer stated that the milestones for the remaining of the year are well thought out and a logical continuation of earlier milestones.

Reviewer 2:
The reviewer noted that there is ongoing work for FY 2019 to focus on the investigation of Li surface protection with organo-sulfide but added that no future work is planned as this is the last year of this project.

Reviewer 3:
The reviewer explained there are some quantitative metrics, but the CE goals are still too low (99.7% is still too low for a practical cell, which needs about 99.95%).

Reviewer 4:
The reviewer commented that the future plans for next year are mainly an optimization of organo-Li_xS_y and organo-$Li_xP_yS_z$ composite Li protection to demonstrate homogeneous Li-metal deposition and improvement of CE to 99.7% for 300 cycles; however, there is no fundamental materials design concept that has been pointed out to achieve the projected target.

Reviewer 5:

The reviewer stated that volumetric efficiency simply must be addressed

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

Reviewer 1:

The reviewer described the project as highly relevant and supportive of DOE objectives to develop an affordable high-energy-density battery for electric vehicles. There is still a challenge to achieve dendrite-free plating and stripping of Li with high-cycling efficiencies. This will be required to achieve long-cycle life required for affordability. The effort is addressing this issue.

Reviewer 2:

The reviewer affirmed that this project strongly supports the DOE new energy competitive objective. Electrochemical energy storage has a broad impact on the U.S. energy landscape and U.S. economy and is a very important program in DOE. The reviewer added that a Li-metal electrode can enable high-energy-density rechargeable battery and a S electrode can significantly reduce battery cost and increase cell energy density. The reviewer concluded that the team has made significant improvements to both systems.

Reviewer 3:

The reviewer said the development of a novel Li-metal host anode without dendrite formation along with identification of high S-loaded electrode configurations (6 mg/cm^2) for use in full-cell Li-S batteries can meet the DOE-targeted energy density of greater than 350 Wh/kg and cycle life of approximately 1,000 cycles for the next-generation EV application.

Reviewer 4:

The reviewer agreed that Li-S batteries support the DOE objectives.

Reviewer 5:

The reviewer remarked that until the volumetric energy density problem is addressed, Li-S is not going to be useful to the automobile industry.

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 resources for this project have been sufficiently utilized and the stated milestones have been achieved on time.

Reviewer 2:

The reviewer replied that the resources are sufficient to achieve the milestones on time.

Reviewer 3:

The reviewer indicated the resources are adequate for the scope of the project.

Reviewer 4:

The reviewer wrote that resources appear sufficient.

Reviewer 5:

The reviewer said resources are adequate.

Presentation Number: bat332
Presentation Title: High Electrode Loading Electric Vehicle Cell
Principal Investigator: Mohamed Taggougui (24M Technologies)

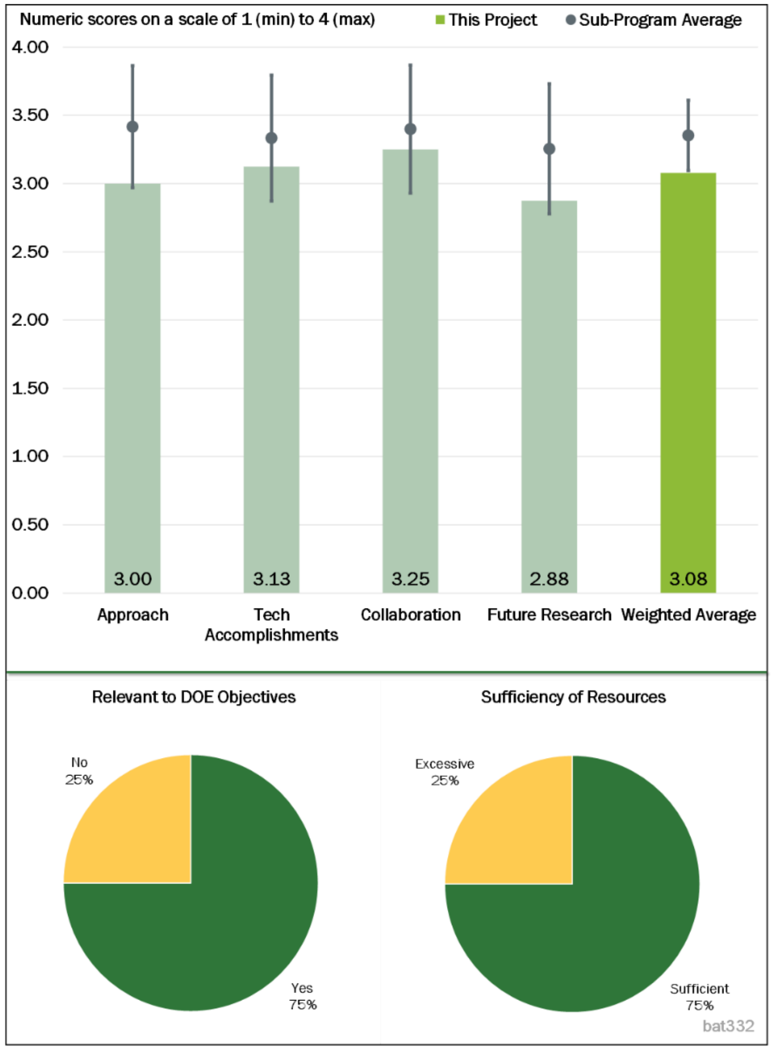

Figure 2-44 – Presentation Number: bat332 Presentation Title: High Electrode Loading Electric Vehicle Cell Principal Investigator: Mohamed Taggougui (24M Technologies)

Presenter
Mohamed Taggougui, 24M Technologies

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

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 approach designed to accomplish the target is reasonable.

Reviewer 2:
The reviewer indicated that it involves semi-solid technology to make thick electrodes with a simplified process.

Reviewer 3:
The reviewer said the cell performance and results are well stated but the approach details are missing.

Reviewer 4:
The reviewer wrote that the approach to develop and demonstrate 24M's manufacturing technology to make cells with thick electrodes appears appropriate. Achieving larger scale cells appears to have been successful but achieving performance targets that are relevant to automotive applications is lacking.

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 project progress was planned and accomplished well.

Reviewer 2:
The reviewer found that the PI's team successfully demonstrated thick electrodes of NCM-811 cathodes and realized a 500-cycle life with a capacity retention of approximately80%. It would be great, the reviewer added, if the PI's team can provide more detailed characterization on the structure of the electrodes after cycling.

Reviewer 3:
The reviewer indicated that NMC-811 achieve 500 cycles with 80% retained capacity.

Reviewer 4:
The reviewer wrote that as the project is nearly complete, 24M has demonstrated cells using the unique semi-solid manufacturing process. However, the reviewer found that the key metrics that are relevant to automotive applications have not been met. Achievements in cycle life and overcharge protection are clear. Power performance and fast charge are not adequately explored but can be assumed to be poor based on the electrode thickness. While electrode thickness is significant (300-600 µm), the porosity and press density of electrodes is not reported. For automotive applications, volumetric energy density is more important than gravimetric, yet neither reported energy density is revolutionary and neither meets or comes close to the DOE targets of 350 Wh/kg and 750 Wh/L.

The reviewer elaborated that flexibility of the manufacturing method to work with other cell formats and still achieve high energy density should be explored. For safety testing, overcharge alone is not an adequate validation of the safety profile (i.e., should include oven and nail penetration or autoclave testing). The demonstration of the Si-hybrid anode concept is not convincing and needs much more validation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said collaboration within the team appears appropriate to complete the upcoming cell testing.

Reviewer 2:
The reviewer wrote that the full cells were tested by ANL, which is appreciated, and added that SNL performed the abuse testing to verify the cell performance, comparing it with the target performance.

Reviewer 3:
The reviewer stated the collaborators' roles are clear.

Reviewer 4:
The reviewer said there is wide project collaboration with several National Laboratories, academia, and industrial companies.

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 wrote that the future research may test the cycling under different thermal conditions.

Reviewer 2:
Some suggested items from the reviewer were to increase the charge (C) rate as C/3 is still not enough, extend the cycle life, and understand the mechanism of low C rate and the poor cycle of the semi-solid cell. The reviewer asked if this is related to the electrode configuration (semi-solid and thick electrode).

Reviewer 3:
The reviewer commented that the PI's team will work on the targets of Phase 3, including cells with energy density of 350 Wh/kg, fast charging at a current rate of 4C, and demonstration of low-temperature operation. The detailed proposed methods were not clearly stated.

Reviewer 4:

While the project is nearly complete, the reviewer concluded that there is significant effort needed to create a competitive automotive cell through the 24M manufacturing process. Unfortunately, the reviewer wrote, there are no concrete suggestions made on how to achieve these targets.

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

Reviewer 1:

Yes, the reviewer wrote, the development of thick cathodes with a high areal capacity is highly needed to further improve the cell energy density.

Reviewer 2:

The reviewer stated that Li-ion batteries with high energy density and long cycle lifetime are important for electric vehicles.

Reviewer 3:

The reviewer noted that the project aims to develop high-energy-density, low-cost Li-ion battery, which is related to DOE objective.

Reviewer 4:

While this project does address the goal of advancing alternative manufacturing strategies for EV battery cells, the reviewer said it does not meet the most basic criteria for cell performance that would lead to adoption of the 24M technology. There is no significant impact on energy, power, and abuse tolerance, nor are there convincing calculations regarding cost (other than that for capital expenditures).

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

Reviewer 1:

The reviewer indicated that the PI's team well demonstrated pouch cells in terms of performance. It would be great if more characterizations on the electrode structure can be provided.

Reviewer 2:

The reviewer stated that the tasks and milestones are completed.

Reviewer 3:

The reviewer commented that resources are enough for the proposed research.

Reviewer 4:

The reviewer remarked that the total project cost to DOE appears excessive based on the demonstration results. There are many cells that can achieve similar or better performance parameters even without thick electrodes. Without a demonstration of the disruptive nature of the manufacturing technology, the reviewer wrote, the cost seems high.

Presentation Number: bat338
Presentation Title: Extreme Fast Charging Cell Development Overview
Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

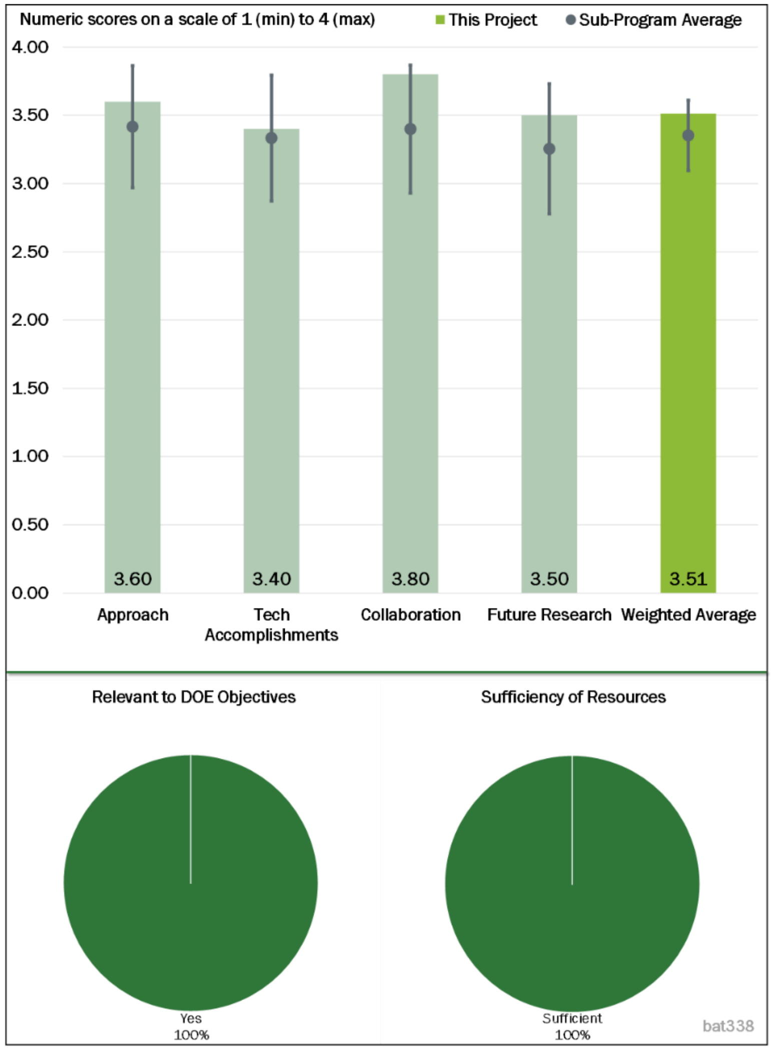

Figure 2-45 – Presentation Number: bat338 Presentation Title: Extreme Fast Charging Cell Development Overview Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

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 noted that this project is one of a series of projects that aim at understanding the cell degradation mechanisms due to fast charging. This is a critical step to set the limit of fast charging and to design electrodes to enable fast charging. The project integrates a broad range of technical approaches, ranging from cell design, characterization, modeling, and advanced diagnostics methods, which are necessary to address the technical barriers. The well-integrated results point out the importance of inhomogeneity amplified by the short charging time.

Reviewer 2:
The reviewer described the approach to perform work as very methodical. Because there are so many variables, output can be obtained in XRD (in terms of lithiation) or discharge capacity when designed experiments have all input paraments (e.g., charging rate 1C /7C, thin/thick, cycle number, NMC composition, voltage, silica, porosity, tortuosity). This technique, sometimes called DOE Taguchi fractional factorial design, can significantly reduce the number of trials.

Reviewer 3:
The reviewer wrote that the combination of all sub-projects in this activity is well focused on this important area and is providing timely and valuable findings.

Reviewer 4:
The reviewer said the Xcel program addresses one of the biggest challenges of EV adoption. The program defines challenges at multiple timescales and length-scales, and the questions that the project team is attempting to answer would be a solid foundation to solve issues related to fast charging.

Reviewer 5:
The reviewer observed that this approach is communicated as a combination of electrode construction, testing, advanced characterization techniques, and numerical modeling. The reviewer agreed that this is required for this problem and applauded the project team effort that is currently underway.

The reviewer suggested several areas of improvement. The first is a greater focus of just before and just after the onset of Li plating. The experiments should move in the direction of identifying the initial onset SOC for plating for a specific test condition and then not charged any higher. The observation of extreme Li plating is okay for the start of the project, but this really is a sign that the experiment was poorly planned. Greater precision is required. The second suggestion was to use of a "controlled anode potential" either through anode potential defined by simulation or by a reference electrode or both. All experiments should be designed based on this knowledge set. The reviewer believed the tools the project team has are sufficient to design much more detailed and clever experiments. The last suggestion was that SiO_x is industrially relevant and found in commercial cells. DOE should perhaps take a more nuanced view of Si having a calendar-life problem. Perhaps low amounts (10% or less) of SiO_x or a highly engineered Si could be included in the project. This is a much more attractive approach to industry, which allows simultaneously for fast charge and high energy density, in contrast to fancy and likely impractical graphite electrode architecture.

Industrial cells have a large amount of self-heating, which greatly helps with fast charging (see work of C.Y. Wang from PSU). This is critically important. There are already some results in this project showing how important temperature is. It would be great if this project sorted out where all of these benefits come from.

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 thought excellent technical progress with very impressive results, macroscopic phenomena to atomic-level insight, has been achieved in this project.

Reviewer 2:
The reviewer wrote that good work is being done. The reviewer particularly appreciated the measurement of concentration profiles within the electrode.

Reviewer 3:
The reviewer stated that the project has made significant progress since its start. The reviewer explained that well-integrated results point out the importance of inhomogeneity amplified by the short charging time. Li plating has been identified as one of the main failure mechanisms and it correlates with the graphite-lithiation state (LiC_6 and LiC_{12}). The reviewer elaborated that the in-situ synchrotron study also revealed that the graphite is not lithiated uniformly through the electrode thickness. This SOC gradient will be more significant during faster charging.

Reviewer 4:
The reviewer found that accomplishments of the combination of projects to date is excellent and appears to be proceeding well. One missing element, which should be included sooner rather than later, is work to understand the impact of cell compression and pressure and/or cell expansion forces, as dependency on these simple mechanical parameters may significantly influence the specific outcome of many of the studies and is important as we consider real-world solutions to fast-charge issues.

Reviewer 5:

The reviewer said the project is still new and only 37% completed so we need to wait but it looks promising.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said the program formed an excellent team and the reviewer found a good use of resources and synergies from the National Laboratories and universities.

Reviewer 2:

The reviewer responded that it appears that everyone is working together and added "Good job."

Reviewer 3:

The reviewer indicated that collaboration of the research team from the different institutions is one of the strengths of the project. The reviewer added that the technical approaches are complementary, and the results are well integrated.

Reviewer 4:

The reviewer stated it seems a good number of team meetings among involved parties are occurring.

Reviewer 5:

Generally, the reviewer wrote, collaboration appears to be and probably must be working well and must be being well coordinated in order to achieve the overall combination of accomplishments and progress to date. However, the reviewer suggested that better illustration of the specific contributions of the university partners may help illuminate the extent of collaboration across 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 described it as generally excellent, and asked the project team to please refer to specific comments for each sub-project in this area. Again, the reviewer urged the project team to plan to include greater work on compression and pressure and/or cell expansion force sooner rather than later as that may be one critical partial-path adjustment.

Reviewer 2:

The reviewer described the approach to perform work as very methodical. Because there are so many variables, output can be obtained in XRD (in terms of lithiation) or discharge capacity when designed experiments have all input paraments (e.g., charging rate 1C /7C, thin/thick, cycle number, NMC composition, voltage, silica, porosity, tortuosity). This technique, sometimes called DOE Taguchi fractional factorial design, can significantly reduce the number of trials.

Reviewer 3:

The reviewer believed the direction of the proposed future work should provide insights into the issues associated with fast charging.

Reviewer 4:

The reviewer suggested a greater focus of just before and just after the onset of Li plating. The experiments should move in the direction of identifying the initial onset SOC for plating for a specific test condition and then not charged any higher. The observation of extreme Li plating is okay for the start of the project, but this really is a sign that the experiment was poorly planned. Greater precision is required.

The reviewer also suggested use of a “controlled anode potential” either through anode potential defined by simulation or by a reference electrode or both. All experiments should be designed based on this knowledge set. The reviewer believed the tools the project team has are sufficient to design much more detailed and clever experiments.

SiO_x is industrially relevant and found in commercial cells. The reviewer suggested DOE should perhaps take a more nuanced view of Si having a calendar life problem. Perhaps low amounts (10% or less) of SiO_x or a highly engineered Si could be included in the project. This is a much more attractive approach to industry, which allows simultaneously for fast charge and high energy density, in contrast to fancy and likely impractical graphite electrode architecture.

Industrial cells have a large amount of self-heating, which greatly helps with fast charging (see work of C.Y. Wang from PSU). This is critically important. There are already some results in this project showing how important temperature is. The reviewer concluded that it would be great if this project sorted out whence all these benefits come.

Reviewer 5:
The reviewer wrote it was not discussed in this project.

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

Reviewer 1:
The reviewer said fast charging is critical for the mass implementation of EVs, which are critical to reducing importation of oil.

Reviewer 2:
The reviewer wrote that the program will provide critical understanding of maximum charging rate for commercial Li-ion chemistry for EVs.

Reviewer 3:
This project is highly relevant to support the overall DOE objectives, the reviewer stated, elaborating that it illustrates the main degradation mechanisms and the contribution of each factor (temperature, rate, electrode design, etc.) The outcome of this project will not only set the limit for fast charging but also give guidelines on how to design batteries for fast charging.

Reviewer 4:
The reviewer noted that DOE and industry are looking into extreme fast charging along with avoiding cell degradation temp rise and Li plating so this is very relevant

Reviewer 5:
The reviewer concluded that it supports progress and understanding toward higher battery energy densities, and/or higher charge rate capabilities for BEV’s.

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

Reviewer 1:
Noting that the program has two more years with well-organized structures, the reviewer expected that the team could answer fundamental understanding, which will advance fast charging of state-of-the-art high energy Li-ion cells (high-nickel TM oxide with Gr-Si composite).

Reviewer 2:
The reviewer wrote that based on the outcome of the project, the resources for the project seems to be sufficient. However, this is a very large research team, and it is not clear how the resources are distributed within the research team.

Reviewer 3:
The reviewer indicated the resources are sufficient.

Reviewer 4:
The reviewer suggested that collaboration with a National Laboratory statistics team who has expertise in designed experiments can be valuable.

Reviewer 5:
The reviewer remarked that the resources for the stated milestones of the specific sub-projects in this area may be sufficient, but a greater number of projects and funding would be beneficial to further accelerate understanding and development in this critical overall area of fast charge.

Presentation Number: bat339
Presentation Title: Impact of Anode Design on Fast-Charge Applications
Principal Investigator: Kandler Smith (National Renewable Energy Laboratory)

Presenter

Andrew Jansen, Argonne National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

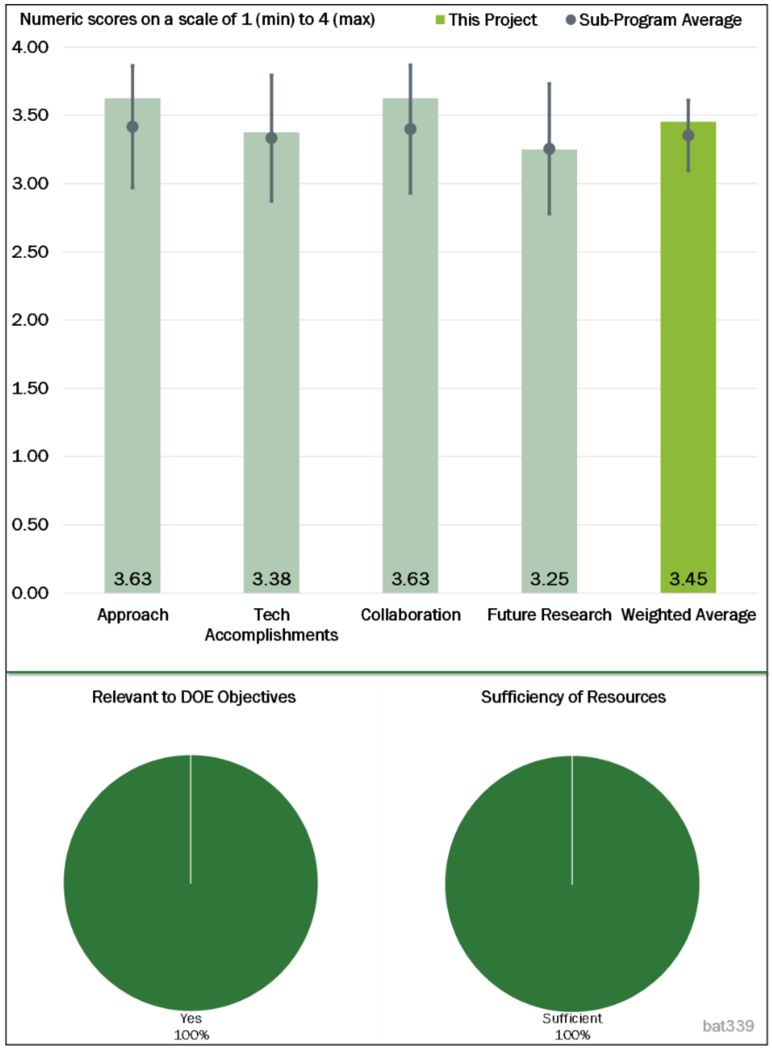

Figure 2-46 – Presentation Number: bat339 Presentation Title: Impact of Anode Design on Fast-Charge Applications Principal Investigator: Kandler Smith (National Renewable Energy Laboratory)

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:

Regarding the approach, the reviewer gave the following comments: Providing a consistent set of electrodes for the entire team to use is a great approach for this project; the development and implementation of a reference electrode, which resides in the middle of the cell, is also excellent; and the experimental validation of concentration gradients across the cell is also very valuable.

Reviewer 2:

The reviewer stated that the program is well designed for a multi-institution deep dive in a way that everybody uses the same electrodes and procedures to address fast-charging problems. The use of NMC-532 with upper cutoff voltage of 4.1V might not reflect real operation conditions; the reviewer understands cycling at 4.1V exclusive positive effects and the focus on graphite anode. However, the reviewer added, damages in cathode particle were observed, and effects become dominant or at least quite substantial in commercially relevant, state-of-the-art Li-ion chemistry.

Reviewer 3:

The reviewer explained that the research team fabricates controlled anodes in pouch cells for the Xcel team to study fast-charging degradation mechanisms. In this review, they showed two cell designs. The round-1 cell has 2 mAh/cm² anode loading and the round-2 cell has 3 mAh/cm² anode loading. They expected this level of loading will allow them to observe the degradation mechanisms during fast charging more clearly.

The reviewer elaborated that several new approaches were developed to address the key technical barriers. They developed a method to quantify a Li-metal on anode via ICP-MS. They also implemented the reference electrodes to identify the point of Li plating. These new approaches provided valuable insights for Li plating during fast charging.

Reviewer 4:

The reviewer explained that the project seems to have a well-focused approach with several important and key areas targeted, including work toward better understanding the impacts of porosity and tortuosity, good three-electrode studies to understand specific electrode polarization contributions, and developing and demonstrating useful methods for plated Li quantification.

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 identified, among other significant accomplishments, the advancement in understanding of porosity and/or tortuosity effects on capacity with rate-dependent cycling, which should inform and encourage further work within this project and across other related projects within VTO.

Reviewer 2:

The reviewer observed that steady process was made according to the plan. They have developed numerous materials, electrodes, and cells for the Xcel team and provided materials and electrochemical data for modeling. This is part of large efforts to understand the cell degradation mechanisms due to fast charging.

Reviewer 3:

Overall, there were impressive progress in loading two different anodes, and it certainly helps to understand plating phenomena during fast charging. Addressing inhomogeneity in graphite electrodes via operando experiments is outstanding. The reviewer wondered whether this set of experiment can be done in positive electrodes too.

The reviewer noted that there was a quite large variations in cell performance in low porosity (26%) and number of particles within electrodes seems to be a cause. Given the fact that tortuosity becomes very critical in highly dense anode, the reviewer suggested making a higher areal capacity design to study an impact of loading and porosity. Also calculating tortuosity values for each electrode would be informative, adding that there are ways to measure tortuosity (symmetric graphite cells, 3-D reconstruction, etc.).

Reviewer 4:

On electrode formulation and loading, the reviewer appreciated the comments made by the presenter, but the fast-charge problem is an electrode- and electrolyte-engineering problem rather than an active materials chemistry problem. It would be valuable if the binder content could be greatly reduced in the electrodes as it likely contributes directly to the electrode impedance. An industrially relevant binder would also be important. It would also be valuable to focus on area-specific capacities 3.5 mAh/cm^2 or greater (based on cathode reversible capacity), which then would provide a minimal acceptable energy density and maximal acceptable cost.

The reviewer suggested that work would benefit greatly from focusing on examining the behavior at anode potentials just above or just below where Li-plating is expected either based on reference electrodes and/or simulations. A constant current charging profile from 0% SOC to 4.1V is of little practical importance. The reviewer said the team has these excellent tools. The reviewer is excited to see the results the team generates by designing more precise experiments from the combination them (R.E. and modeling, etc.).

Noting the role of temperature is clearly shown in these results, the reviewer declared this to be great. However, the reviewer hoped the next year the team will dig down a bit deeper to understand what role this plays.

Small amounts of silicon oxide or an advanced silicon material (less than 10 wt%) could play an important role in simultaneously achieving energy density and fast charge goals. DOE should be out ahead of industrial implementation not behind.

The X-ray work is very interesting, but unclear what the takeaway is. Perhaps it is just too early. The reviewer looked forward to seeing how this develops.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that this is part of large efforts to understand the cell-degradation mechanisms due to fast charging and added that this project is well integrated with the rest of the reach efforts.

Reviewer 2:
The reviewer indicated the program is well coordinated and collaborated within team.

Reviewer 3:
The reviewer found that project appears to show good collaboration across the project team, and the apparent involvement of the specific university partners would be considered excellent, but there is no way to discern in which specific areas the university partners are contributing, and there seems to be no differentiation regarding this for other projects under the same umbrella.

Reviewer 4:
The reviewer affirmed that teamwork is obvious but urged the team to please try to connect modeling and reference electrode work with charging profile development and also with in situ and operando characterization.

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

Reviewer 1:
The reviewer described this as cell focused and targeted, with likely specific and useful outcomes.

Reviewer 2:
The reviewer stated that SiO_x is a much more promising solution than elaborate low-density graphite-based architectures.

Reviewer 3:
Writing that the proposed plans look reasonable, the reviewer remarked that it would be interesting to run even higher loading (greater than 4 mAh/cm2) with high-nickel NMC (-622, -721, or -811) to fully understand the impact of porosity and tortuosity) and the impact of positive materials during the fast-charging procedure.

Reviewer 4:
The reviewer wrote that several interesting observations deserve more mechanistic study and require further explanation. The first observation is that Li plates more with higher anode loading and the anode showed large SOC variation. Therefore, the higher loading effect may be just because of a thicker electrode and more SOC gradient. The project team also noticed that higher temperature leads to less Li plating. This may be because the improved diffusion at higher temperature leads to less SOC gradient. More connections among different observations need to be developed in order to identify the key mechanism. The second observation is that the project team has found the anode potential dropped below 0. The reviewer asked if one can add a reference electrode in the real cell and apply a cutoff voltage just for the anode during fast charging to avoid Li plating.

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

Reviewer 1:
The reviewer concurred that the program fully supports DOE objectives and goals.

Reviewer 2:
This reviewer found that this project is highly relevant to support the overall DOE objectives. It illustrates the main degradation mechanisms and the contribution of each factor (temperature, rate, electrode design etc.). The outcome of this project will give guidelines on how to design batteries for fast charging.

Reviewer 3:
The reviewer stated that fast charging is very important to widespread adoption of EVs in the marketplace.

Reviewer 4:
The reviewer said this project supports progress and understanding toward higher battery energy densities, and/or higher charge rate capabilities for BEVs.

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 while the resources are very significant and appear to be at least sufficient or even beyond sufficient, the output and progress so far, and as planned, seem to be of significant and corresponding value.

Reviewer 2:
The reviewer said the resources seem to be well utilized.

Reviewer 3:
The reviewer noted that the resources are sufficient.

Reviewer 4:
The reviewer wrote that based on the outcome of the project the resources for the project seems to be sufficient but added that it is unclear how resources were distributed in this project.

Presentation Number: bat340
Presentation Title: Impact of Charging Protocols on Cell Degradation
Principal Investigator: Dennis Dees (Argonne National Laboratory)

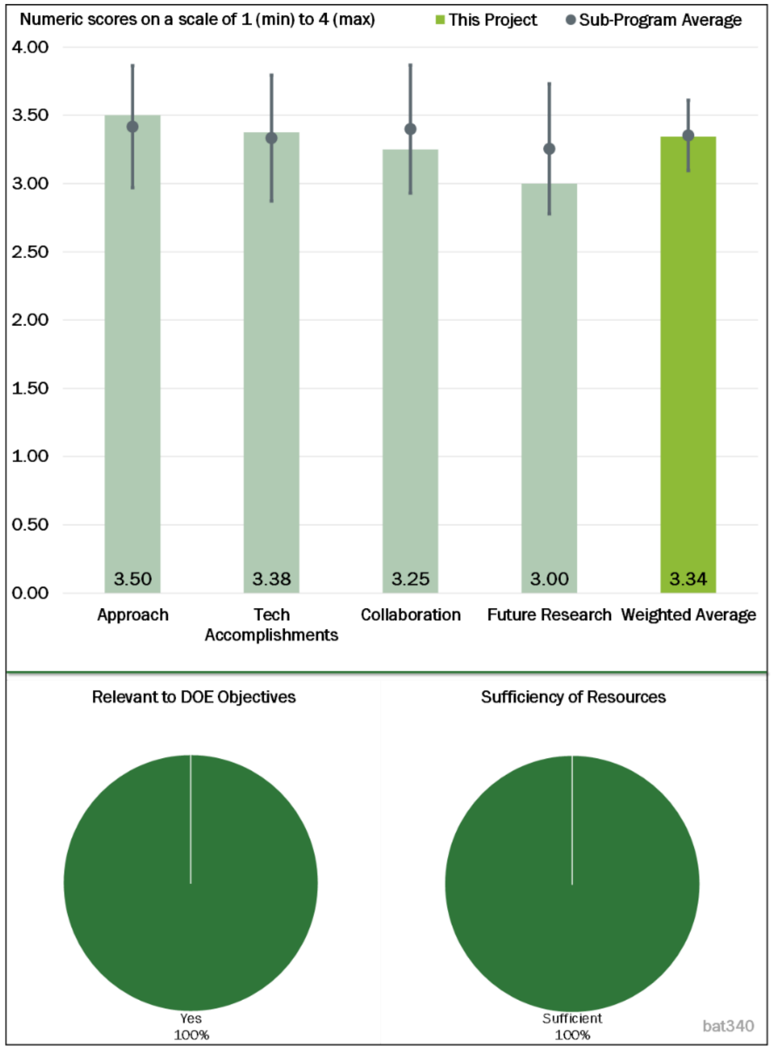

Figure 2-47 – Presentation Number: bat340 Presentation Title: Impact of Charging Protocols on Cell Degradation Principal Investigator: Dennis Dees (Argonne National Laboratory)

Presenter

Erik Dufek, Idaho National Laboratories

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 the project approach has useful targets toward understanding key limitations and parameters in fast charge capability. Part of the specific focus being on protocols is excellent, as is that on the impact of cell variability.

Reviewer 2:

The reviewer remarked that this project focused on using full cells to identify and quantify failure modes, provide insight into materials degradation after cycling, and areas where materials and electrolyte advances can be made. This is an essential part of a large team effort on understanding the cell degradation mechanisms due to fast charging. The reviewer elaborated that the team separated the contributions from the ohmic resistance and transport to the total voltage loss. The reviewer concluded the information is important for cell level of design.

Reviewer 3:

The reviewer affirmed that the project is well designed and feasible. Due to fact that cathode particles showed damage after fast charging protocol (even at 4.1V of cell voltage), the reviewer wrote that it is worth paying more attention to the cathode.

Reviewer 4:

The reviewer remarked that multi-step charging is very important to achieving fast charging without Li plating. However, it would very valuable to have the charging profiles derived from the simulation activities and/or reference electrode studies. The reviewer suggested that this should be the focus over the next year. The use of CE measurements after a fast-charge cycle could perhaps provide an instantaneous measure of loss of cyclable Li. The reviewer added that most cyclers like MACCOR can achieve the precision required without any fancy equipment.

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 made the following three comments regarding technical accomplishments and progress: the first is that quantifying over-potentials and the origins of capacity loss are very important – good work in this area. The second is that establishing the importance of temperature is also good work – keep pushing in this direction. The third is that measurement of cathode cracking and potential for this to be an important fading mechanism is also an important contribution.

Reviewer 2:

The reviewer explained that this project provided degradation mechanisms at the full pouch cell level. The research team reported that the impedance and transport increases with the C rates and the transport showed a different (higher) slope above 7 C. This result is significant, as it may set the limit for fast charging. They also reported cathode cracking as the main degradation mechanism.

Reviewer 3:

The reviewer described the project as having very useful results across a range of multiple focus areas. Greater narrative or clarity in a few cases regarding model versus actual data could be helpful as could greater explanation regarding basis for differences between model and actual data for results where both exist.

Reviewer 4:

The reviewer commented that the conclusion of MS charging procedure is not well defined due to high variability. The reviewer would like to know how to improve variation in this experiment because spending less time in high SOC (or voltage) via MS charging, in principle, will not stress anode.

In addition, cathode fading becomes higher at high C-rate and high areal capacity; correlation among capacity fading contribution of each electrode-areal capacity needs to be understood thoroughly. The reviewer also wondered whether there is depth dependency in particle fracture (e.g., more damage close to separator or current collector).

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that collaboration looks very strong and sufficient.

Reviewer 2:

The reviewer wrote that this is part of a large effort to understand the cell-degradation mechanisms due to fast charging, adding that it is well integrated with the rest of the project team.

Reviewer 3:

The reviewer remarked that the project appears to show good collaboration across the project team, and the apparent involvement of the specific university partners would be considered excellent, but there is no way to discern in which specific areas the university partners are contributing, and there seems to be no differentiation regarding this for other projects under the same umbrella.

Reviewer 4:

The reviewer stated that numerical models and/or reference electrode studies should be directly used to determine optimal charging profiles.

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 future research looks good and adequate to cover next year and implementing an electrolyte system with better transport property proposed by modeling will be very informative. The reviewer said it is also important to work with an industry partner (if there is any) to establish relevant cell chemistry, experimental design, etc.

Reviewer 2:
The reviewer suggested that the project could benefit from some consideration and inclusions for (1) bulk cell or specific electrode thickness expansion, and/or (2) cell pressure changes, and/or (3) impact of applied cell compression forces on degradation, and the interactions or dependency of any of these factors with charging protocol.

Reviewer 3:
The reviewer remarked that the proposed future research is more diverging than converging. The reviewer elaborated that it is not clear if Li-plating still an important degradation mechanism at the cell level from this report. If it is not, then the reviewer asked why it is not. The reviewer also wanted to know what causes the difference in the Li-plating amount in this study and that observed in project BAT339. Further quantification of the degradation mechanisms may be helpful to sort out what is more important.

Reviewer 4:
The reviewer stated it is not clear how this proposed future work fits within the other proposals from partner projects. The reviewer suggested more focus should really be put on "Impact of Charging Protocols on Cell Degradation" rather than the stated future work in the presentation (more mechanistic analysis). A great deal more could be achieved through protocol development than what was communicated.

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

Reviewer 1:
The reviewer found that this project is highly relevant to support the overall DOE objectives. It illustrates the main degradation mechanisms, adding that the outcome of this project will set the limit for fast charging.

Reviewer 2:
The reviewer indicated the project supports the DOE objectives very well.

Reviewer 3:
The reviewer wrote that fast charging is critical to increase the share of EVs in the marketplace.

Reviewer 4:
The reviewer said the project supports progress and understanding toward higher battery energy densities, and/or higher charge rate capabilities for BEVs.

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 while the resources are very significant and appear to be at least sufficient or even beyond sufficient, the output and progress so far, and as planned, seems to be of significant and corresponding value.

Reviewer 2:
The reviewer concluded that the team seems to have enough resources to achieve the project objectives.

Reviewer 3:
The reviewer wrote that funding seems appropriate.

Reviewer 4:
The reviewer stated that it is not clear how resources were distributed in this project.

Presentation Number: bat355
Presentation Title: Development of High-Performance Lithium-Ion Cell Technology for Electric Vehicle Applications
Principal Investigator: Keith Kepler (Farasis Energy)

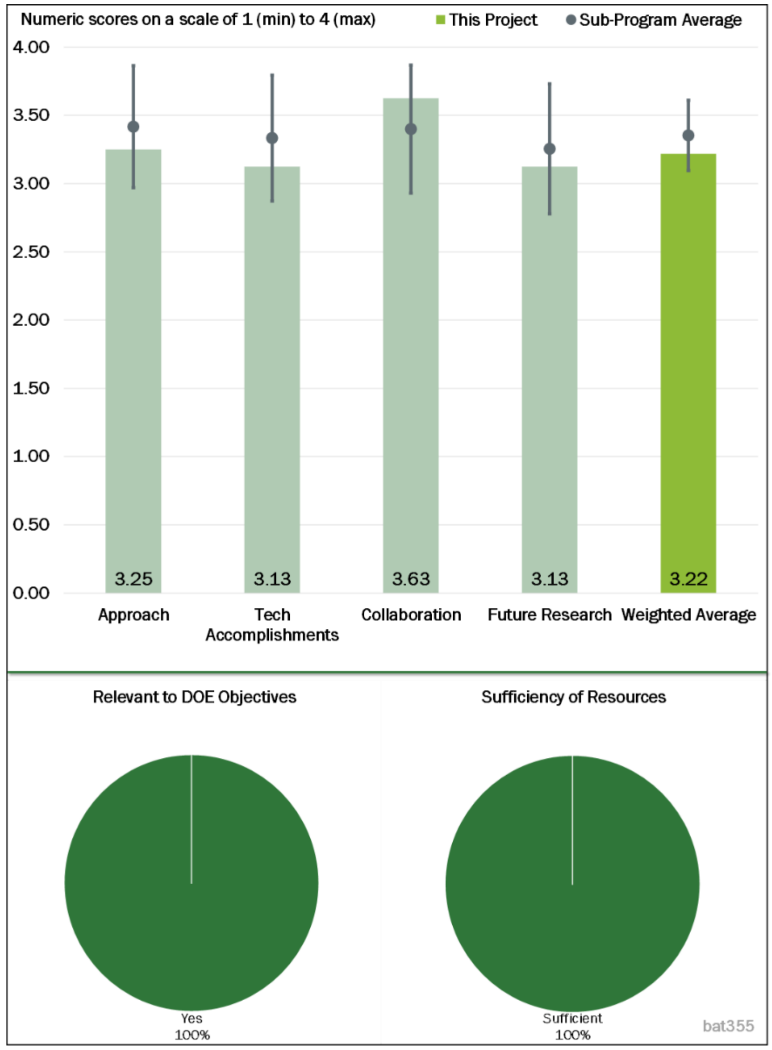

Figure 2-48 – Presentation Number: bat355 Presentation Title: Development of High-Performance Lithium-Ion Cell Technology for Electric Vehicle Applications Principal Investigator: Keith Kepler (Farasis Energy)

Presenter

Keith Kepler, Farasis Energy

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 found that the approach appears excellent, adding there is good organization and testing protocols. Use of cells at different scales is well done. The reviewer concluded that DOE barriers are being addressed in cell development of increasing scales.

Reviewer 2:

The reviewer affirmed that the project is designed well as evidenced by the tests done on the system to check its performance. Calendar life at full state of charge is particularly demanding.

Reviewer 3:

The reviewer praised the project as extremely well organized but added that science is not cooperating on the anode side while there is a lot of progress on the cathode.

Reviewer 4:

The reviewer remarked that the approach to this project seems to be simply varying material parameters in a Si - NMC cell to optimize performance and reach the revised target of 330 Wh/kg by the end of the project. The reviewer said that it is unclear how this straightforward approach to cell optimization will be successful where others have failed—in particular in addressing the issues of Si volume expansion, Ni-rich cathode stability, etc. Simply trying harder and turning more knobs is not very convincing—especially not when multiple materials are all being changed at once. It is difficult to assess the effect of any one change when so many improvements are being pursued at once—especially when the data are mostly on the system-level performance. Confidence in the system performance will not be reached by demonstrating 330 Wh/kg for a set of test cells; that confidence will only come if you understand the individual material contributions involved in getting to that demonstration. That said, the reviewer concluded that this project is serving as a systems integrator for several materials development at the National Laboratories and in industry. As a result, all performance data that are being collected will have some value in evaluating the potential of many of these materials “advances” in a real-world cell, even if it is not as definitive as it could be. The reviewer also noted the project responded to previous reviewer comments and added calendar life testing, which is helpful.

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 indicated that the work has progressed well in terms of cell builds with improved capacity.

Reviewer 2:
The reviewer remarked that cathode progress very good and slides were convincing on project management side. However, the reviewer added, there was not a lot of optimism on the silicon anode. Everything associated with the cycling was good, but the project team was very upfront that the storage stability was their concern along with silicon deterioration without cycling. The reviewer was surprised that the slides did not directly address this barrier and what the project team was trying to do to overcome it.

Reviewer 3:
The reviewer indicated that the project is making reasonable progress in performance targets at the full cell level—and the project team will likely be able to demonstrate 330 Wh/kg by the project’s end. But there is scarce evidence that the project is making process on the challenges to control and stabilize Si-volume expansion, increase cathode stability, reduce Li consumption and capacity loss, etc. These material challenges are listed on Slide 21. Reaching the prototype goal of 330 Wh/kg implies that at least some of these challenges have been met or partially met, but more direct evidence of progress toward the specific material challenges underlying the performance goals at the cell level would be desirable.

Reviewer 4:
The reviewer concluded that the results reported are focused on the Gen1 cells but based on the project plan timing it appears substantial reporting of work on Gen2 cells should also be done. The reviewer observed that it is clear the goal of 400 Wh/kg has been changed to 330 Wh/kg, but again, this reviewer did not see many results on how work toward cells at 330 Wh/kg is going. The progress on the Gen1 cells appears good, but that only brings the team more or less up to the Li-ion baseline.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted that there are a lot of contributors to this project at the materials level, and the primary contractor is managing well the coordination aspect across the various contributors. Just keeping the project on schedule with Gen1 development and testing was quite a feat. The reviewer praised the excellent job.

Reviewer 2:
The reviewer said that exchange of cells with National Laboratories for independent validation was done for example showing good collaboration and coordination.

Reviewer 3:
The reviewer affirmed this is a well-managed project with lots of organizations and companies involved. Clearly, the project management team is in control. The reviewer noted as a minor point that the presentation did not spell the company’s name correctly.

Reviewer 4:
The reviewer stated that other team members are mentioned, although it is hard to tell how well integrated the members are.

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 the plan is moving forward with plans in place and the future research looks good.

Reviewer 2:
The reviewer commented that the proposed research is more like goals than a research plan. However, the problems are appropriately identified.

Reviewer 3:
The reviewer wrote that notwithstanding the suggestion that having more data on the individual effects of new material incorporation would have been desirable, the proposed future work is very appropriate given where the project is today. The plans for Gen2 development and testing are consistent and logical. The reviewer found that the schedule is also very reasonable and likely to be met. The only curious thing for the reviewer is why the project team will continue exploring LFO as a Li source when they have ruled it out for Gen2 cells and revised the target capacities for these cells based on that decision. Perhaps further LFO development for this project is a "No-Go." The reviewer added that the future plans are also not clear on what if anything will be done to address the high-temperature calendar life issue that has been identified but this is less of a concern.

Reviewer 4:
The reviewer said that there are not many details on how exactly the team will achieve cells at 330 Wh/kg and how far the testing has come along.

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

Reviewer 1:
The reviewer found clear alignment between the project's goals to leverage materials improvements in prototyping a high energy density, long-life Li-ion cell with DOE objectives and performance targets for battery development to support vehicle electrification.

Reviewer 2:
The reviewer affirmed that this project is directly pushing vehicle battery technology and seeing how far we can tweak the NMC technology. The reviewer added that this the type of project that is needed with a maturing technology. Any breakthrough on the anode side will be able to vault battery technology when combined with this work.

Reviewer 3:
The reviewer stated that the goals of higher energy density, lower cost, and longer cycle life are supported by this program.

Reviewer 4:
The reviewer wrote that this fits with the DOE goals.

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

Reviewer 1:
The reviewer said this is a big project funding from many directions. It is a lower risk project that is maturing NMC technology. The reviewer said such a project could use more funding; however, there must be a balance.

Since total funding is limited, there has to be money for the less mature and higher risk projects as well. Given the balance, this is well funded.

Reviewer 2:

The reviewer wrote that given the planning and coordination that occurred in Gen1 cell development and testing, the resources in the project appear to be sufficient to complete the future work on schedule as proposed.

Reviewer 3:

The reviewer affirmed that based on the steady progress toward the objectives the funding levels seem sufficient.

Reviewer 4:

The reviewer indicated resources appear sufficient.

Presentation Number: bat356
Presentation Title: Lithium-Ion Cell Manufacturing Using Directly Recycled Active Materials
Principal Investigator: Mike Slater (Farasis Energy)

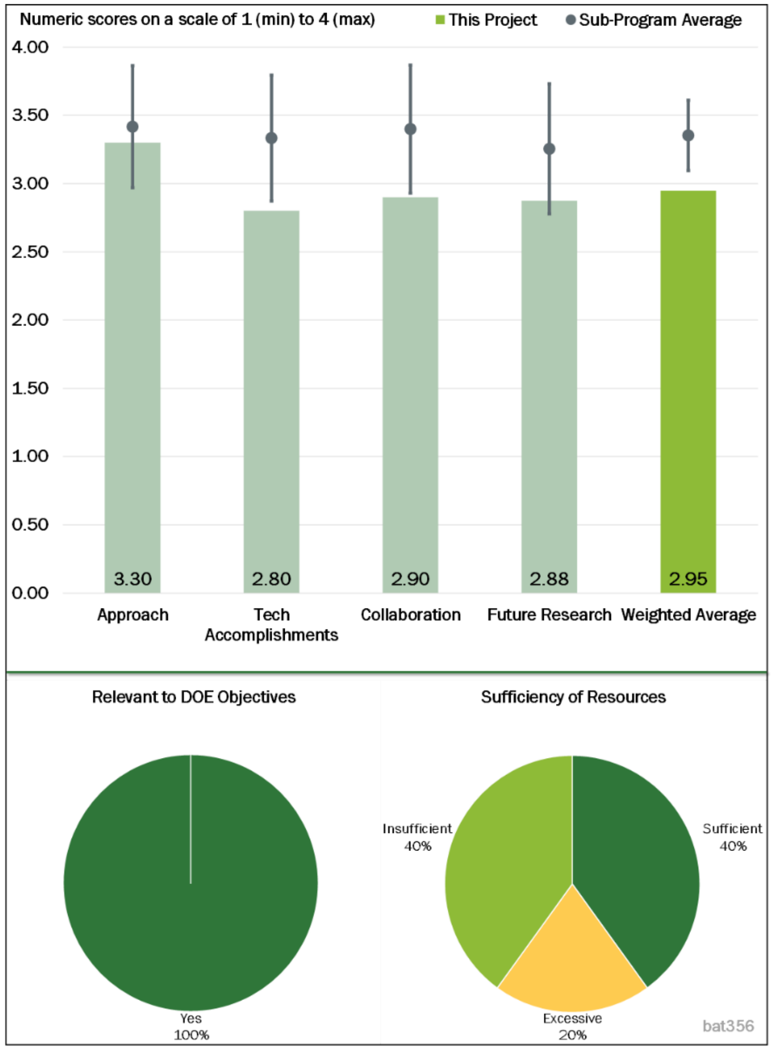

Figure 2-49 – Presentation Number: bat356 Presentation Title: Lithium-Ion Cell Manufacturing Using Directly Recycled Active Materials Principal Investigator: Mike Slater (Farasis Energy)

Presenter
Mike Slater, Farasis Energy

Reviewer Sample Size
A total of 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 approach appears reasonable, although it appears that substantial delays have been encountered and the project expenditures are well behind schedule. The reviewer indicated it sounds like both technical and organizational issues are limiting the rate of progress.

Reviewer 2:
The reviewer said the program is progressing well and the performance of the recycled materials is good, adding that technically it appears to be feasible. There is not enough information to judge whether this is an economical approach.

Reviewer 3:
The reviewer remarked that the primary technical barriers they aimed at were overcome but the remainder of the battery was not recycled, which was not a goal of their project.

Reviewer 4:
The reviewer explained that the project focuses on the recovery of the value-containing materials from the battery and battery material scrap via the direct recycling process. It includes also the issues of quality and variability of the feedstock, which probably is the most challenging issue of direct recycling. It was not completely clear to the reviewer if the process will be supporting the battery production facility, thus the feedstock will be relatively uniform, not obsoleted, or if the process t will be used for recycling end-of-life (EOL) spent batteries. In the latter case, the issue of high variability of the feedstock and obsolete chemistries should be expected.

Reviewer 5:

The reviewer stated that the general approach to evaluating direct recycling processes for Li-ion battery materials was reasonable and would have produced valuable test data on two cycles of 1 Ah pouch cells from ANL and FEI, but clearly not enough contingency was built into the approach to account for possible delays in process development and cell manufacturing. With the benefit of hindsight, the reviewer suggested it would have been better to limit the approach to fewer feedstock and processing variations and perhaps to only one round of pouch cell testing. In the end, the approach proved to be not quite feasible given the schedule and/or budget resources allocated to the 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 indicated that Slide 11 presents key results, but it was a little hard to interpret. First, the testing is in coin cells, which really give only limited information. It is unfortunate that much larger cells are not tested; this likely reflects the challenges in the project. Also, the figure does not have a label for virgin graphite and virgin NMC- 111, so the baseline is not clear. The reviewer noted that there are two lines for recycled graphite/recycled graphite that are much different, and asked for the reason. Also, all these cells show quite poor capacity retention, so comparing among all bad cells is not very helpful.

Reviewer 2:

The reviewer indicated that the outcome in terms of performance is quite good but added that many of the milestones are delayed.

Reviewer 3:

The reviewer suggested that it looks like they fell behind many times. The reviewer could not tell if all items had been addressed from project sheet and is unsure if this is a presentation flaw or incomplete tasks. The reviewer added kudos in that the team delivered the #1 goal of working batteries with performance exceeding the controls.

Reviewer 4:

The reviewer commented that this rating contains two components: strictly technical one— on excellent level—and the progress of the project—much weaker, caused by the delays. The reviewer elaborated as follows regarding the technical issues: recovering 1-2-kilogram (kg) quantities of the materials does not allow one to fully assess the method performance and quality of the output materials against the feedstock variability, unless the feedstock was a specially prepared mix, which is not stated. Cycle-efficiency evolution would be more interesting instead of first-cycle efficiency. The reviewer wanted to know what can be expected the recovery yield of the optimized process for rNMC. Regarding the delay issue, the reviewer commented that despite the fact that the majority of the time has already passed, the advancement of the project is poor. Out of the 20 milestones only 6 are completed and one is 50% done.

Reviewer 5:

Despite the delay of pouch-cell testing, the reviewer stated that there was progress on process development and coin-cell testing. Although demonstrated by others, the project showed that NMC cathode material can be recovered with the material structure largely intact and can further have its Li content readjusted to the point that the material actually outperforms virgin material in coin cells. The reviewer said it is not clear what "opportunistic material engineering during recycling may be responsible for improved performance characteristics" means, so progress on understanding the fundamental chemistry in the recovery process may or may not have occurred. Also, while the data on trace element contamination (specifically, F^-) from the PVDF binder decomposition) are valuable, the real effects of these elements versus virgin material would have been better understood with the more rigorous testing that was planned for the pouch cells. In summary, some progress was made on the goals of the program, but it is difficult to see how much more progress can be made in the time remaining in this no-cost extension phase of the project. Perhaps elemental data for recycled material from whole cell processing will become available along with initial coin cell cycling, which would be helpful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer wrote that it sounds like the collaborations were helpful but not sufficient.

Reviewer 2:
It was not clear to the reviewer how much collaboration is ongoing but it appears to be okay. The reviewer suggested that more specific notation of where characterization data are sourced would be helpful to answer this question.

Reviewer 3:
The reviewer remarked that the project team had to based on the results.

Reviewer 4:
The reviewer noted that the project collaborates with LBNL. The reviewer suggested that possibly more collaborations would help to keep momentum in the project.

Reviewer 5:
This is a repeat concern from the previous review, the reviewer wrote, but the project likely would have made more progress with additional collaborators for characterization other than just LBNL. Although the project cites that they have increased informal collaborations at other institutions, it was not clear to the reviewer just what these other collaborations are and how they have (or have not) been beneficial over the past year since the last review. The reviewer added that collaboration with LBNL itself was fine.

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 presenter did a good job of presenting barriers, such as a diverse waste stream. This should not be a major issue until aftermarket batteries hit the market—and so before that hits, DOE should get ahead of the pack to have industrialized standards for marking that would preclude that from happening.

Reviewer 2:
The reviewer suggested a bit more focus on existing results might be beneficial before looking at additional feedstock. The reviewer added it would be logical to choose high=value feedstocks.

Reviewer 3:
The reviewer found that the proposed future research covers well the remaining barriers. The reviewer suggested that the project should make an effort to speed up cell manufacturing at a pilot facility.

Reviewer 4:
The reviewer remarked that it is hard to tell if the plan is to complete the goals of the original project or pivot to other topics, such as looking at other cell chemistries.

Reviewer 5:

The reviewer observed that because the project has ended and is technically in a no-cost extension phase until October, there are limited options for any future work based on the project's current assessment of being 66% complete. If pouch cells can be obtained and tested in this timeframe, then getting any reasonable data on such cells should be a priority for the time remaining. If not, it could be somewhat valuable to complete the initial evaluation of the cathode material recycled from whole cell feedstock as the materials characterization data (tap density, F) content, etc.) suggest that it might be somewhat different from the material from the electrode-only feedstock.

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

Reviewer 1:

The reviewer affirmed absolutely, noting that vehicles must be recycled. The reviewer elaborated that 10 million new vehicles per year means almost that many retired every year. Additionally, batteries are unique and contain precious metals and toxic chemicals.

Reviewer 2:

The reviewer indicated that the project's primary goals to develop direct recycling processing for Li-ion cells and modules clearly support DOE objectives to ensure a critical supply of active materials for the next generation of electrical energy storage for vehicle applications.

Reviewer 3:

The reviewer stated that the project focuses on direct recycling, which can recover with highest efficiency the remaining value of the feedstock and contribute to highest extent to the sustainability requirements.

Reviewer 4:

The reviewer wrote yes, elaborating that the program may enable lower cost based on discussions with the PI and also mitigate concerns about limited resources such as Co, NI, and Li.

Reviewer 5:

The reviewer said this is aimed at 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 explained that this project is in a no-cost extension phase and there is clearly not enough time or budgetary resources to achieve the originally stated goals for the project. Some of the remaining resources should be committed to finalizing the data and conclusions that are achievable and then perhaps disseminating these results in either a technical presentation at an international conference and/or in a published journal.

Reviewer 2:

The reviewer suggested the resources might be borderline insufficient based the delays in the program, but sufficient progress has been shown toward these program goals.

Reviewer 3:

The reviewer commented that either the timeline was a little impractical, personnel or equipment was unavailable, or the funding a little on the low side. Since the reviewer did not oversee the project (and did not ask the question), it is impossible to assess which it was or something else.

Reviewer 4:

The reviewer stated that it appears this team has not been able to spend the funds.

Reviewer 5:

The reviewer noted significant project delays indicate the resources were not appropriate or the project organization was not optimal.

Presentation Number: bat357
Presentation Title: Thicker Cathode Coatings for Lithium-Ion Electric Vehicle Batteries
Principal Investigator: Stuart Hellring (PPG)

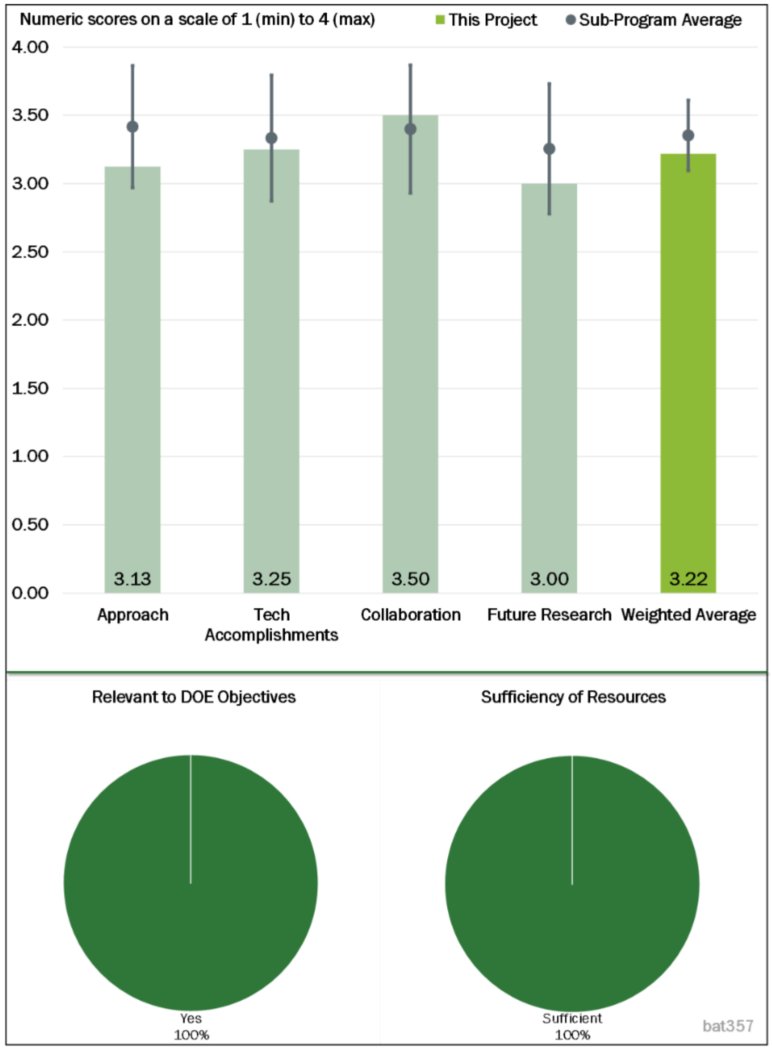

Figure 2-50 – Presentation Number: bat357 Presentation Title: Thicker Cathode Coatings for Lithium-Ion Electric Vehicle Batteries Principal Investigator: Stuart Hellring (PPG)

Presenter
Stuart Hellring, PPG

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 agreed that the results are promising, and the approach seems sound to demonstrate proof of concept for new binder and solvent formulation with improved properties compared to NMP.

Reviewer 2:
The reviewer remarked that there has been good progress on a problematic project. The reviewer elaborated that the presentation seems overly focused on peel strength over battery performance. The reviewer added that peel is obviously an advantage of this technology as well as mixing, stability when mixed, and drying speed over that of PVDF.

Reviewer 3:
The reviewer stated that the approach appears well organized, and various partners are included to make progress in the work. However, the reviewer added that It is somewhat hard to tell exactly what the approach is due to the proprietary nature of the additives.

Reviewer 4:
As is common with testing and optimization of a complex system of materials, the reviewer explained that the approach is structured around several different sets of test cells with increasing cathode thickness starting with “Baseline” cells at about 22 mg/cm^2 to “1st Target” cells at about 30 mg/cm^2 and finally “Final Target” cells at 40 mg/cm^2. Although the goal to get to cells with thick (40 mg/cm^2) cathodes is clear, the reviewer remarked that it is less clear what the evaluation metrics will be once these thick cells are fabricated and tested. The desire to maintain flexibility and adhesion in the thick cathodes is clearly stated, but the electrochemical performance targets for the project are not. It is simply implied that the thick cathodes should electrochemically be at least equal to the “Baseline” cells with 22 mg/cm^2 cathodes. The reviewer explained

that the problem with this general qualification approach is that the “Baseline” versus “1st target” versus, “Final Target” is not being rigorously controlled – that is, there is no standard anode being used for all. Cells are being manufactured and tested at different places, and there is a significant risk of “apples versus oranges” comparison being drawn.

Strictly speaking, the reviewer elaborated, it appears that the “Baseline” cells that have been delivered to INL contain the optimized PPG binder, so that the performance comparison of “Baseline” versus. “Final Target” will only allow a comparison of thickness of that binder–and not its performance relative to commercial grade NMP-processed binder. This limit in the approach will also limit the impact of the results.

The reviewer suggested the approach would have been better if it had included cathodes made with NMP- and non-NMP-processed binders at the various thicknesses with all cells made by the same facility and tested by the same laboratory. Said another way, just because you show data for one cell configuration made by one laboratory and tested in one way that shows better performance for PPG binder cathode versus NMP-based binder (e.g., Slide 12), the reviewer cannot draw the conclusion that under all future configurations, combinations of electrode materials, and with manufacturing and testing done in all ways, that one binder will be always better than the other. To do so, risks “apples to oranges” comparisons and occasionally misleading conclusions.

As a final note, the reviewer indicated it would have been good to have some electrochemical characterization of the cathode material’s electronic and ionic conduction with the new binders. In the end, these two parameters limit the thickness of cathodes to thicknesses where diffusion is not a problem. Flexibility and adhesion matter, but so does charge transport.

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 indicated that performance data look very promising for the thick electrode, but added it might be interesting to note any changes in the formation process, if any, are needed.

Reviewer 2:

The reviewer noted that the presenter identified many causes of variation that might be holding the project back. The reviewer is unsure if everything can be blamed on materials supplied.

Reviewer 3:

Despite some concerns about the approach noted above, the reviewer concluded that the project has made significant progress so far–particularly by demonstrating new binders with good flexibility and adhesion. The adhesion (peel test) and flexibility radius (1/8” radius) are impressive, even if these parameters do drop off (e.g., ½” radius) with the thicker cathode films. Similarly, the reviewer stated, there is evidence that the binders may help with capacity retention, even though it appears that the new binder formulations have a much lower capacity on first cycle–at least when the binders are used in anode fabrication (Slide 9). For cathode fabrication, the reviewer observed that the binders appear to produce high-capacity retention (Slide 12), but here the anode is not specified, and it is not clear that the anode is the same as the “Baseline” cells delivered to INL. It would be helpful if the team only used the term “Baseline” to refer to the specific 14 cells delivered to INL in the fourth quarter of FY 2018. The reviewer added that it is confusing to hear that “Baseline” and “1st Target” cells are being produced at the University of Michigan Energy Institute (UMEI), but that PSU’s contribution to the project includes “assemble baseline pouch cells with existing anodes at PSU to screen cathodes for deliverables to INL.”

Reviewer 4:

The reviewer stated that it is somewhat hard to tell exactly what has been achieved. The reviewer pointed out that the goal is 40 mg/cm^2 cathodes, but there are no data from testing such cathodes. It sounds like thick cathodes may be made on a pilot line, but it is not clear if they have good properties. There are no electrochemical results. The actual results appear to be for much more standard loadings.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that the program has a diverse and appropriate set of collaborators, adding that a clear description of the work being done was provided.

Reviewer 2:

Clearly, the reviewer said, they are addressing issues important to all the groups and working together.

Reviewer 3:

The reviewer commented good use of UMEI for coatings, but added that it is not clear how involved LG is at this point.

Reviewer 4:

The reviewer reflected that after bringing in PSU to collaborate on the anode development, it is not clear why PPG will now revert to developing the thicker cathodes in their own laboratory for the “Final Target” cells. In the end, collaboration across the team appears to be been beneficial, but perhaps not optimal. The reviewer also remarked that the project is now faced with trying to complete all three phases of the test cells in the final few months of the project–with baseline testing the furthest along and final target testing awaiting anode development. The reviewer concluded that it just seems that the project could be farther along with better coordination and collaboration earlier in the project.

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

Reviewer 1:

The reviewer stated that future research plans appear well funded, but added that it sounds like significant work remains.

Reviewer 2:

The reviewer commented that the proposed future research is appropriate but there is not a lot of detail.

Reviewer 3:

The reviewer remarked that the project team is switching directions in the second half of the project, so it is difficult to answer this question. The reviewer offered that the team did a good job with the solvent-based electrode and will be repeating similar issues with the water-based electrode in the second half of the project. The reviewer said it remains to be seen if the technical issues with the solvent-based electrode can be fully solved by the end of the project. If this were a go-no-go point in the project, this reviewer would say, “GO.”

Reviewer 4:

The reviewer commented that the project is nearing completion so the remaining work to be done is fairly obvious, but added that there is a lot of work still to do. The reviewer elaborated that the plan for thick anode development at PPG is completely unclear, and the progress on the final target cells will certainly be impacted. The reviewer suggested it might be wise to formulate a contingency plan for maximizing the impact and value of comparing baseline cells to first target cells only–being able to draw the most complete conclusions–with the assumption that final target cells might not be available due to the remaining hurdles for that set of test cells.

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

Reviewer 1:
The reviewer found that the project's primary goal of developing and validating electrochemically a non NMP-processed binder for a Li-ion cell that additionally has the flexibility, adhesion, and charge-transport characteristics to enable much thicker cathode and anode formulations is clearly aligned with DOE objectives to achieve higher capacity, higher power, and safer rechargeable batteries.

Reviewer 2:
The reviewer said it is focused on DOE goals.

Reviewer 3:
The reviewer stated that it addresses need for safer, environmentally sounds way to fabricate a Li-ion battery, but added it is difficult to determine how it will performance under a high rate

Reviewer 4:
The reviewer commented that DOE needs to fund alternative manufacturing and not just new materials, otherwise the battery business will only be imported into the United States.

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 appropriate resources are committed.

Reviewer 2:
The reviewer said the project seems to be on target with the funding it is given.

Reviewer 3:
The reviewer replied that resources appear sufficient.

Reviewer 4:
The reviewer responded that the remaining budgetary resources and schedule are likely sufficient to complete both the baseline-testing phase and the first target-cell tests. Beyond that, however, the reviewer suggested the resources may be too thin to achieve the final target cells as originally conceived, but only time will tell if that is the case.

Presentation Number: bat365
Presentation Title: Stabilizing Lithium-Metal Anode by Interfacial Layer
Principal Investigator: Zhenan Bao (Stanford University/SLAC National Accelerator Laboratory)

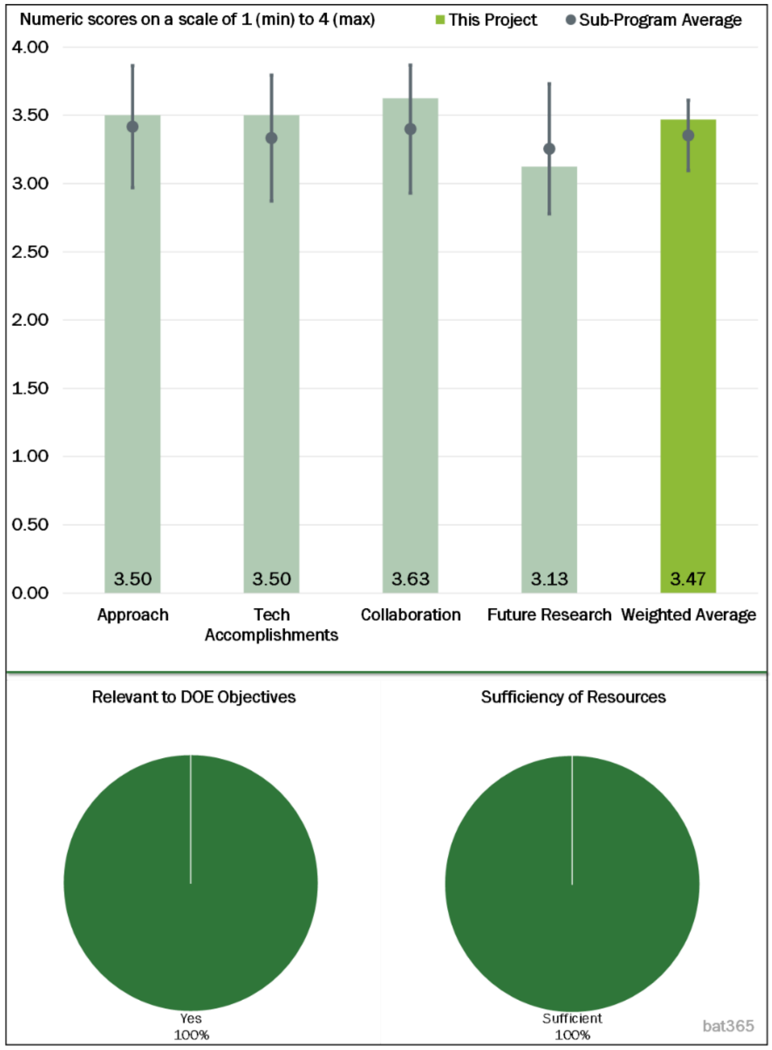

Figure 2-51 – Presentation Number: bat365 Presentation Title: Stabilizing Lithium-Metal Anode by Interfacial Layer Principal Investigator: Zhenan Bao (Stanford University/SLAC National Accelerator Laboratory)

Presenter

Zhenan Bao, Stanford University/SLAC National Accelerator 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 found that the effort is logical and addresses key issues confronting a long cycle-life Li anode. The reviewer added that it is good that two strategies will be explored, the first being engineering interfacial protection materials and the second being developing Li-host materials, as this will improve the chance for success.

Reviewer 2:

The reviewer remarked that the approach is to use soft polymer interfacial layers at the Li-electrolyte interface in order to increase cycle life by preventing Li dendrites and side reactions.

Reviewer 3:

The reviewer replied that the interplay among critical parameters and chemical reactivity solvation polymer dynamics for polymer design is important and a designed experiment by statistical technique will be valuable.

Reviewer 4:

The reviewer indicated that the approach to the project is clearly designed to overcome the technical barriers associated with the safe and reliable use of Li metal as an anode in high-capacity Li-ion batteries. Although the approach is focused correctly, the reviewer suggested that the project may need to adjust the current approach to have a reasonable chance of reaching the difficult and perpetually elusive goal of stabilizing a Li-metal anode during plating and stripping with near-perfect cycling efficiency. Recently, the reviewer noted, limited model studies (e.g., adhesion energy versus plating morphology and solvent Li-ion solvating power versus. plating morphology) have been used by the project team to develop desirable characteristics of the protection layer for the Li metal–that is, stable to Li, in constant contact with the Li-metal surface, and low Li^+ coordination. The reviewer observed that this science-based materials development approach can lead to innovative ideas as to what to try next; this particular problem has repeatedly proven to be resistant to this basic approach–despite the science-based innovation that has been applied to materials engineering of a solution.

The reviewer further indicated that the current project still has enough project time to adjust its approach and add careful modeling and experimentation to specifically identify the source of cycle inefficiency and Li-inventory loss with the basic self-healing polymer (SHP) coating (or close derivatives). If successful, the additional insight and knowledge should accelerate the pace of innovation and progress toward meeting all of the requirements simultaneously. The reviewer added that it should be noted that this project team (almost uniquely) has a tremendous array of synthetic, advanced characterization, and theoretical tools at its disposal. The list of characterization tools alone is world leading. The reviewer suggested that the approach of designing and testing a series of multi-functional copolymers (a H-bonding self-healing hard block and a softer block with the proper Li-ion solvation and surface adhesion) may seem like the best way to go, but asked whether these materials will be any less subject to the coupled mechano-electrochemical processes that underlie the source of the observed cycle inefficiencies.

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 replied that the milestones were met and considerable insights into the roles of polymer mechanics and polymer chemistry on Li-metal deposition were obtained and will help direct future efforts.

Reviewer 2:
The reviewer stated that the project certainly has made progress in the past and continued that trend in the current project year. The reviewer elaborated that past demonstrations of the value of self-healing coatings in dramatically improving the Li-plating morphology have been important and had impact on Li-ion technology. The more recent results on the effects of Li-ion solvation and polymer surface energies on Li-metal deposition have incrementally added to that impact. The concern, said the reviewer, is that the progress has perhaps reached a plateau, particularly in regards to improvement in cycling efficiency. The reviewer concluded that it is clear that the project team has prioritized progress on cycling efficiency going forward, which should help increase the chance of the project reaching its final performance goals by the end of the project in 2020.

Reviewer 3:
The reviewer wrote no comment, adding that, so far, 50% has been completed.

Reviewer 4:
The reviewer responded that current progress has developed a polymer design that combines low reactivity, low Li^+ solvation, and flowable property to improve upon Li cycling. But the reviewer added that the CE of 90% is too low, as agreed upon by the principal investigator.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer stated that it seems excellent collaborations among SLAC teams.

Reviewer 2:
The reviewer pointed out that collaboration is with Professor Jian Qin (Stanford), Professor Steve Chu (Stanford), and Dr. Michael Toney (SLAC) with everyone supporting the effort.

Reviewer 3:
The reviewer found that good collaboration exists between the PI and SLAC (M. Toney).

Reviewer 4:

The reviewer responded that the degree of collaboration among project team members has been very good, especially between Bao and Cui, noting that virtually all of the publications involve those two team members as authors. The reviewer said that there is an opportunity to increase the collaboration with SLAC (Toney) which, as noted earlier, has a vast array of sophisticated characterization tools. That said, the collaboration here is strong and leads to innovative ideas.

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 replied that the milestones for the remainder of FY 2019 are well thought out and a logical continuation of earlier milestones, adding that in FY 2020 there will be an investigation of flowable single-ion conductors.

Reviewer 2:

The reviewer stated that interplay among critical parameters and chemical reactivity solvation polymer dynamics for polymer design will be important since the project is 50% completed, adding that we need to see and wait. The reviewer also indicated that scaling up from a coin cell and a pouch cell will be important for commercial applications.

Reviewer 3:

While it is clear that the team will explore block copolymers as a multi-functional protection coating for Li-metal anodes, the reviewer said it is difficult to provide an assessment of the future work beyond that (FY 2020) because almost no details were presented. In fact, the reviewer noted, the presentation materials simply stated "to further improve the Coulombic efficiency of Li-metal cycling in both ether and carbonate electrolyte" as future work. The reviewer stated that more specificity about how that would be approached would have be helpful. Given that operando characterization has been very impactful in energy storage science and technology, it is difficult to see how useful cryo-TEM will be in understanding the SEI and its effect on Li^+ transport and Li and Li^+ electrochemistry, but it might have been more apparent with more details provided. The reviewer acknowledged that the presentation was admittedly short with only 15 minutes allocated.

Reviewer 4:

The reviewer concluded that further studies are necessary to maintain a stable SEI when cycling metallic metal at high areal capacity. Future research includes systematically varying the dynamics of the polymer, but the reviewer noted that the approach to doing this was not included in the presentation. The reviewer also observed that the active components in the polymer will be decreased to improve CE and limit side reactions, but they are not able to be eliminated entirely. The reviewer remarked that it seems this may be a fatal flaw with this polymer system.

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

Reviewer 1:

The reviewer found this effort as highly relevant to the DOE objectives because it seeks to develop stable, high-capacity Li anodes that will enable the next-generation Li-metal batteries.

Reviewer 2:

The reviewer noted that the protection of Li metal is clearly a high-priority technical barrier that is very relevant to advancing electrical energy storage according to the DOE performance roadmaps. The reviewer added that the project is very well aligned and directly supports DOE objectives.

Reviewer 3:
The reviewer commented that this project is developing an advanced interface that could enable Li-metal electrodes and thereby increase the cell's energy density, adding that this higher energy density will then result in a decrease in cost based on dollars per kilowatt-hour.

Reviewer 4:
The reviewer responded that the DOE goal of avoiding lithiation and stable anode has been followed in this project.

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

Reviewer 1:
The reviewer commented that the resources allocated to the project are clearly sufficient to make progress on the technical goals by the end of the project and provide a more than reasonable chance of reaching the ultimate goal of developing a polymeric interfacial layer for stabilizing Li-metal anodes.

Reviewer 2:
The reviewer replied a good collaboration among the teams suggests that the project has sufficient resources.

Reviewer 3:
The reviewer stated that the project team has sufficient resources to achieve the stated milestones in the time allotted.

Reviewer 4:
The reviewer said the resources are sufficient for the proposed tasking and that the budget is reasonable.

Presentation Number: bat370
Presentation Title: Advanced Diagnostics of Nickel-Rich, Layered-Oxide Secondary Particles
Principal Investigator: William Chueh (Stanford University/SLAC National Accelerator Laboratory)

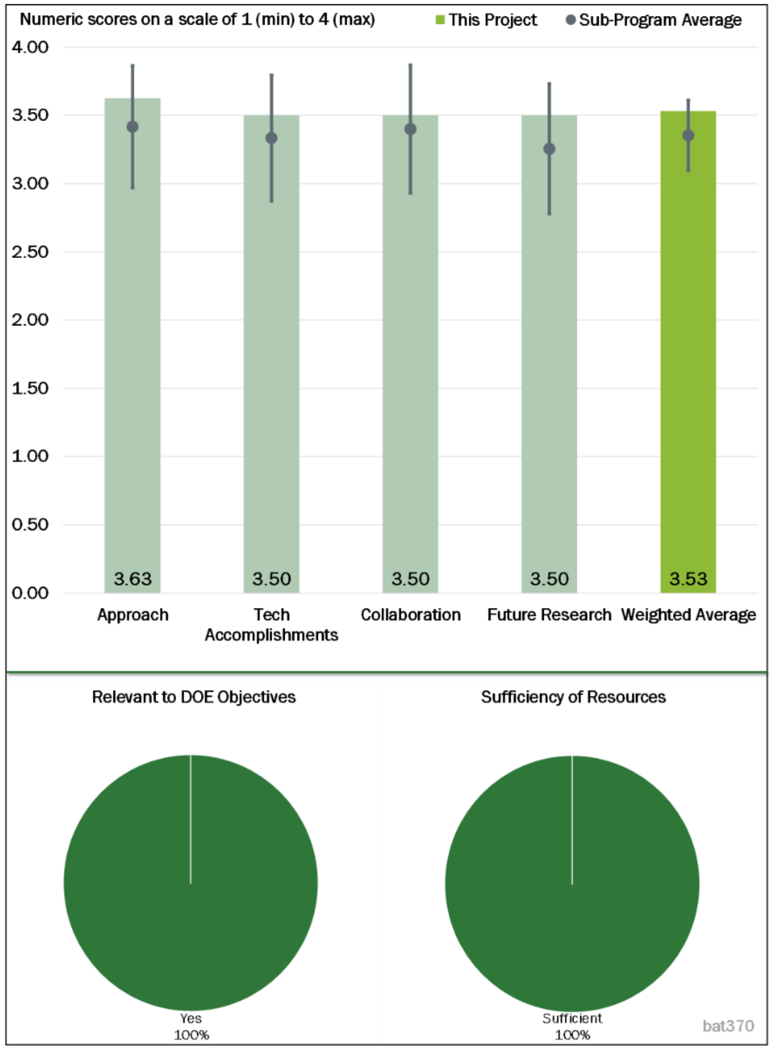

Figure 2-52 – Presentation Number: bat370 Presentation Title: Advanced Diagnostics of Nickel-Rich, Layered-Oxide Secondary Particles Principal Investigator: William Chueh (Stanford University/SLAC National Accelerator Laboratory)

Presenter

William Chueh, Stanford University/SLAC National Accelerator 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 explained that multiple in-situ and ex-situ synchrotron processes were developed to investigate the structure of Li-rich cathodes at different length scale. The reviewer added that correlation of spectroscopy data with microscopy data revealed good information on the structural change of cathode materials during cycling.

Reviewer 2:

The reviewer responded that the approach is to predict failures in batteries using advanced in-situ diagnostics and the objectives are to understand the lithiation and delithiation mechanisms. The reviewer elaborated that the approach is to understand mechanisms in redox (oxygen redox) and how it relates to voltage and capacity decay, chemo-mechanic properties, and what creates hotspots and how to mitigate this. Today, the reviewer said, the approach is looking at the anion-redox work. The reviewer added that the approach is to develop in-situ and ex-situ spectroscopies to relate local chemistry to battery electrochemical characteristics, do meaningful microscopy and spectroscopy experiments, and correlate all the work with macroscopic measurements.

Reviewer 3:

The reviewer stated that the project has developed advanced in-situ or ex-situ diagnostic technology to understanding factors that determine the rate capability and degradation mechanisms of the layered cathode materials that are well designed and feasible.

Reviewer 4:
The reviewer replied that in-situ diagnosis helps to pinpoint and predict battery failure, adding that it will be good to use coin, pouch, and bigger cells to understand phenomena, which can or may occur in battery-management system. The reviewer said that the comparison with impedance spectroscopy as advanced diagnostic tool will be or can be beneficial.

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 the local in-situ X-ray diffraction to reveal local microstructure change as amazing and noted that the oxygen redox model was explained.

Reviewer 2:
The reviewer commented that overall technical accomplishments and progress are good, and reported the following on the Li- -manganese rich(LMR) NMC composite cathodes redox mechanism: order to disorder of the lattice through transition-metal migration; showing the differential capacity (dQ/dV) curve to show the cationic and anionic redox mechanism; it is interesting that the oxygen redox flips on the opposite side; the results show that it is not reversible on the discharge; the project team's theory showing that the transition-metal migration creates a vacancy; relate in a semi-quantitatively; used a model system to look at anion redox; and link structure to electrochemistry.

Reviewer 3:
The reviewer stated that with the combination of X-ray spectroscopy and X-ray diffraction, the anion redox mechanism, as well as migration of transition-metal ions, were confirmed during the cycling LMR transition-metal oxides. A correlation between the voltage fade and the anion redox was established.

Reviewer 4:
The reviewer noted that almost half of the project has been completed, which meets the requirement of the project.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer observed an excellent collaboration between SLAC teams.

Reviewer 2:
The reviewer stated that the team has shown great use of their collaborators as shown by the work presented.

Reviewer 3:
The reviewer affirmed good collaboration, adding that partners participate and are well coordinated.

Reviewer 4:
The reviewer said the team makes good use of several national user facilities but added that on materials side, the collaboration can be expanded.

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 replied that the future work is to transition to in-situ work. Current work was looking at ex-situ work. This is a good approach for the project.

Reviewer 2:
The reviewer wrote that the PIs have planned three future plans, which could effectively meet the requirements of the project.

Reviewer 3:
The reviewer noted that more fundamental issue related to LMR-NMC will be further explored, and techniques for single particle-level diagnosis will also be developed.

Reviewer 4:
The reviewer responded that work on NMC hot spots to stress gradients and particle orientations can be beneficial and that quantification of anion-cation redox will be beneficial. The reviewer also said that a planned matrix of future research with input output variables can be beneficial. The reviewer concluded that the goal should be more pouch level to reflect real-world scenario.

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

Reviewer 1:
The reviewer affirmed that the content of the research is highly related to the objectives of DOE for developing high-energy-density Li-ion batteries.

Reviewer 2:
The reviewer replied that this work is a good fundamental study to help improve cathode performance.

Reviewer 3:
The reviewer indicated that the PIs have developed and utilized a correlative microscopy platform to investigate the electrode materials, which are critical to the design of a safer and more durable battery. The reviewer said that the technology developed in the project will support the overall DOE objective.

Reviewer 4:
The reviewer stated that the DOE goal of advanced diagnostics before anything happens is important in terms of electrode stability.

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

Reviewer 1:
The reviewer replied that the PIs have the necessary equipment and other resources to do the planned experiments.

Reviewer 2:
The reviewer stated the team has sufficient recourses for the project to be successful.

Reviewer 3:
The reviewer said the resource is sufficient to carry out the work.

Reviewer 4:
The reviewer suggested a partnership with GM, a start-up, and universities can help to broaden the research.

Presentation Number: bat371
Presentation Title: Understanding Electrode Scale and Electrolyte Effects During Fast Charge
Principal Investigator: Andrew Jansen (Argonne National Laboratory)

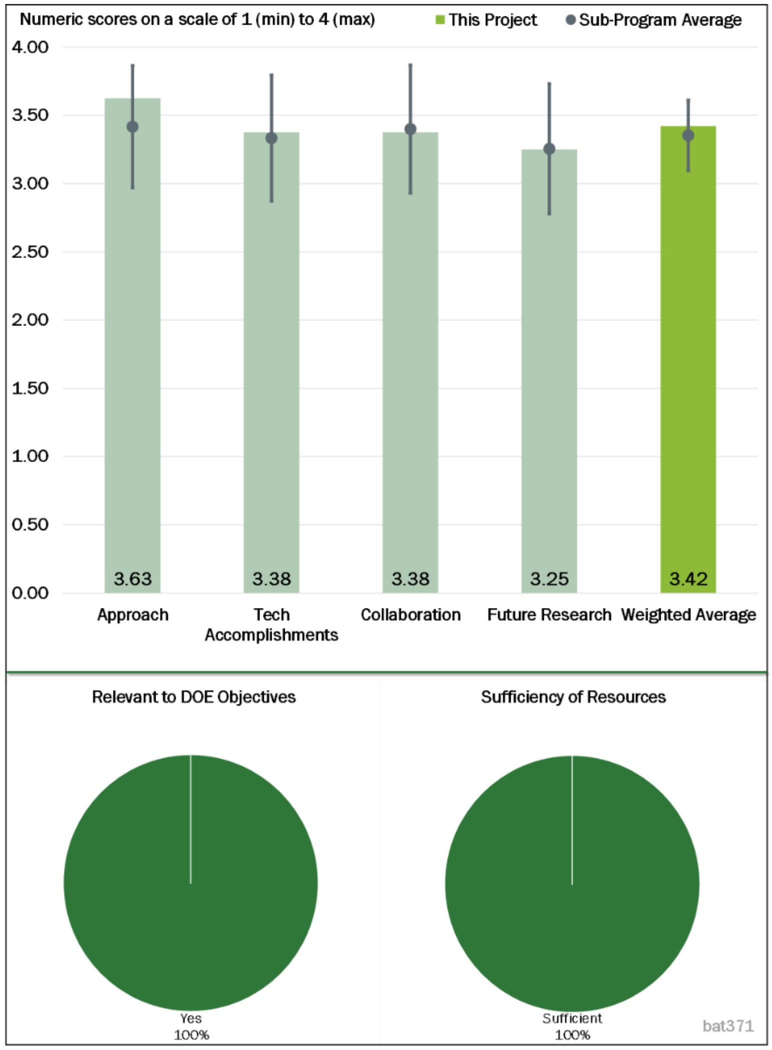

Figure 2-53 – Presentation Number: bat371 Presentation Title: Understanding Electrode Scale and Electrolyte Effects During Fast Charge Principal Investigator: Andrew Jansen (Argonne National Laboratory)

Presenter
Dennis Dees, 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 described the approach as excellent, adding that continuum-scale modeling is the right tool to support the fast-charging goals. The reviewer said the focus on parameter determination and transport properties is worthwhile. Identification of electrolytes with higher transport properties, which also meet all other requirements, is also a great approach.

Reviewer 2:
The reviewer replied the project is well designed and is an important piece of information to understand limiting factors in fast charging.

Reviewer 3:
The reviewer explained that this project focuses on developing electrochemical models to examine transport, reaction, and phase change in graphite-based electrodes and seeks solutions for fast-charge applications. The reviewer added that this is an essential part of a large team effort to understand the cell-degradation mechanisms due to fast charging.

The reviewer explained that the model and experiments comparison can illustrate if there is any gap in the current model. Currently, the model parameters were obtained by fitting experimental data. The data need a bit more rationale. It was not clear to the reviewer why the best fit comes with the activation energy for the solid phase diffusion coefficient (D_S) and exchange current (i_o) of 0 kilojoules per mole (kJ/mol). The reviewer asked what it means for the diffusion and charge transfer reaction. The reviewer said it is important that we learn from the current model and parameters in order to build our confidence in their predictions.

Reviewer 4:
The reviewer said the project approach seems to have useful targets to understand key limitations in fast-charge capability. Specific intent regarding understanding relative impact of porosity versus that of tortuosity seems quite valuable. It was unclear to the reviewer from the results shown whether these are model-only results or actual cell 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 offered the following three observations, the first being on macro-scale porous electrode modeling where the reviewer found solid results. The reviewer suggested it might helpful in the future to study and report how the limiting current of the electrolyte changes as a function of separator, negative electrode, positive electrode, and electrolyte properties. This would allow for a systematic study that separates the transport from the current distribution (competition between interfacial and electrolyte) within the negative electrode. Looking at different temperatures (as was reported) is very useful. It is completely realistic to think of 45 C charging. The second observation dealt with improved electrolytes where, applauding the approach, the reviewer said it might also make sense to evaluate some electrolytes already developed for low-temperature applications (i.e., talk to the National Aeronautics and Space Administration [NASA] Jet Propulsion Laboratory [JPL]). JPL also has completed a huge amount of work on Li plating. They should be able to help the team. For the third observation, which dealt with the graphite phase change and diffusion coefficient, the reviewer called this great work, elaborating that graphite is the most important electrode material and deserves continued attention. The reviewer will be interested to see how this unexpected diffusion behavior is implemented into the model.

Reviewer 2:
The reviewer replied that the technical accomplishments and progress toward the overall project are good, adding that the team obtained good prediction to experimental data and proposed strategies to improve fast charging. The reviewer suggested it might be useful to predict behavior of state-of-the-art Li-ion chemistry (with NMC -622 or -811 with graphite at 4.2-V charge) to elucidate behavior as a future work.

Reviewer 3:
The reviewer noted that several important processes were made. One of the most interesting results is the model pointed out the important properties the electrolyte should have and therefore can suggest electrolyte formulation.

Reviewer 4:
The reviewer found very useful findings and accomplishments across a wide ranging but good set of target areas. The reviewer was unclear if Slides 13 and 14 represent model-based results or actual cell-data results, and it would have been helpful if there had been a clear indication of this. In any case, the reviewer said consideration of impacts of tortuosity, porosity, N:P electrode ratio, temperature, and electrolyte all on one page is very useful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found good teamwork, adding that it is clear that people are talking and working together.

Reviewer 2:
The reviewer concluded that the project team collaboration for the modeling project is good and utilizes the synergies among National Laboratories and universities.

Reviewer 3:
The reviewer stated that this is part of large team efforts to understand the cell-degradation mechanisms due to fast charging, adding that this is well integrated with the rest of the research efforts.

Reviewer 4:
The reviewer remarked that the project appears to show good collaboration across the project team, and the apparent involvement of the specific university partners would be considered excellent, but there is no way to discern in which specific areas the university partners are contributing, and there seems to be no differentiation regarding this for other projects under the same umbrella.

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 but added that including behavior of state-of-the-art chemistry would be useful too.

Reviewer 2:
The reviewer commented that the intention to study cycling performance under high charge rates should be especially helpful future work.

Reviewer 3:
The reviewer said it was the logical extension of presented work. The reviewer also urged consideration of earlier comments for additional future work.

Reviewer 4:
The reviewer wrote that the team has recognized that it is important to include a more detailed SEI model during Li-plating modeling. The reviewer suggested that a recent article (citation: Energy Environ. Sci., 2019, 12, 1286-1295) may be of interest to the research team on SEI modeling and that this may enhance the modeling capability.

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

Reviewer 1:
The reviewer found that this project is highly relevant to support overall DOE objectives, elaborating that the outcome of this project will not only set the limit for fast charging but also give guidelines on how to design electrolytes for fast charging.

Reviewer 2:
The reviewer remarked that fast charging is critical to bring EVs to the broader public.

Reviewer 3:
The reviewer affirmed that the project encompasses all the DOE objectives.

Reviewer 4:
The reviewer said it supports progress and understanding toward higher battery energy densities and/or higher charge rate capabilities for BEVs.

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 while the resources are very significant and appear to be at least sufficient or beyond, the output and progress so far, and as planned, seems to be of significant and corresponding value.

Reviewer 2:
The reviewer concluded that there are sufficient resources allocated to carry out this research.

Reviewer 3:
The reviewer said they are sufficient.

Reviewer 4:
The reviewer stated that it is not clear how many resources were distributed to this project.

Presentation Number: bat373
Presentation Title: First-Principles Modeling and Design of Solid-State Interfaces for the Protection and Use of Lithium-Metal Anodes
Principal Investigator: Gerbrand Ceder (University of California at Berkeley)

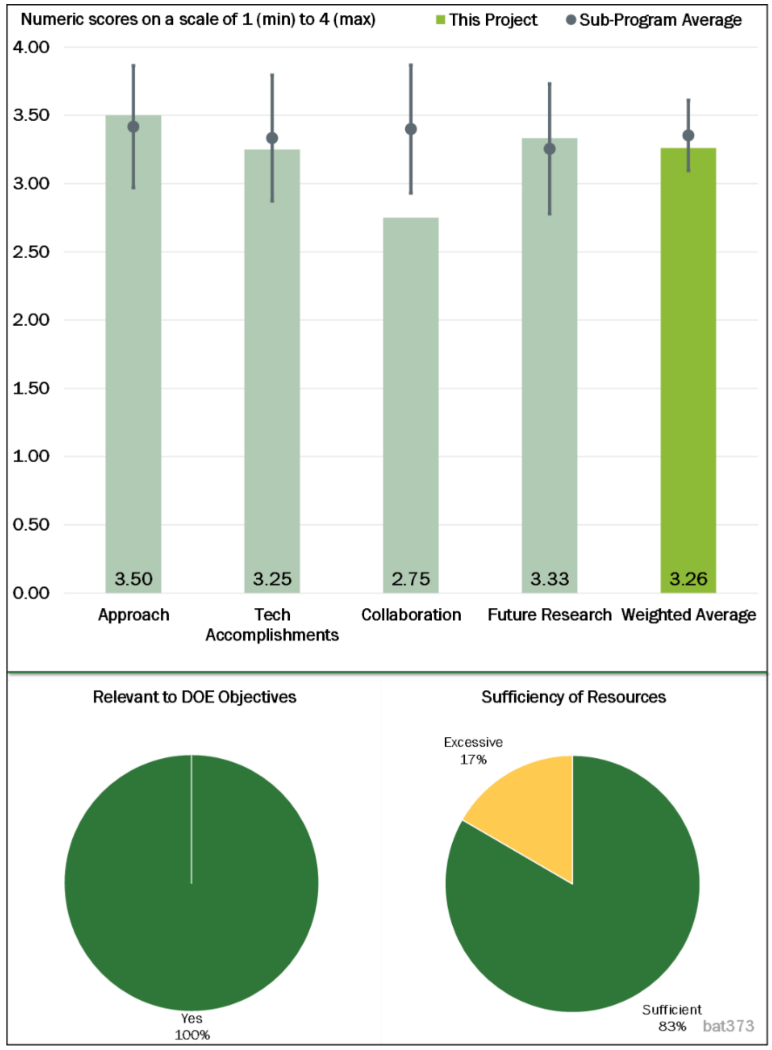

Figure 2-54 – Presentation Number: bat373 Presentation Title: First-Principles Modeling and Design of Solid-State Interfaces for the Protection and Use of Lithium-Metal Anodes Principal Investigator: Gerbrand Ceder (University of California at Berkeley)

Presenter

Gerbrand Ceder, University of California at Berkeley

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 found that the technical barriers, such as ionic conductivity of the solid-state electrolytes, as well as propagation of Li dendrites in the solid electrolytes, are addressed very well, and the progress made in the project clearly demonstrates its good design and feasibility.

Reviewer 2:

The reviewer stated that the technical barrier is being addressed appropriately.

Reviewer 3:

The reviewer explained that the approach to identify high-ionic transport and good electrochemical stability is based on ab-initio high-throughput modeling via calculation of activation barriers for ion hopping, whereas the interfacial mechanical stability is addressed via continuum models. The reviewer found that the proposed approaches are reasonable but the goals of high-ionic transport and high-interfacial stability may be incompatible in some cases. Nevertheless, the reviewer wrote, Li-dendrite growth mechanisms, mechanical effects near the surface, current-density concentration at sharp defects, and pressure effects on Li ion (Li^+) diffusion are well addressed in this project. The procedure is well designed, starting from computational methods for calculating minimum energy paths in different anion prototypes to describing the mechanism of reaction and select nitrides with structural advantage for conductivity. Then, the project team used the continuum model to study the Li-metal dendrite propagation in pre-existing defects to understand Li^+ redistribution at the interface. Finally, the reviewer stated that in the case of the selection of materials with high Li-ionic conductivity, it would be excellent if other databases could also be used.

Reviewer 4:
The reviewer stated that this project adopts a combined approach, which includes a high-throughput materials screening (ab initio modeling) for solid electrolytes with high ionic conductivity and electrochemical stability, and a macro-scale continuum model (including mechanics, electrochemical, and transport) to study the potential for dendrite penetration of such solid electrolytes. The highlight is high throughput screening for such solid ion conductors.

Reviewer 5:
The reviewer suggested that the team take into consideration the visco-plastic behavior of Li at room temperature when modeling stresses and fracture of solid electrolytes caused by Li dendrites. The reviewer provided citations of three recent publications that may be helpful:

Sooraj Narayan and Lallit Anand, "A large deformation elastic–viscoplastic model for lithium," Extreme Mechanics Letters 24, 21-29 (2018).

Erik G. Herbert, Stephen A. Hackney, Violet Thole, Nancy J. Dudney, and P. Sudharshan Phani, "Nanoindentation of high-purity vapor deposited lithium films: A mechanistic rationalization of diffusion-mediated flow," J. Mater. Res. 33 (10), 1347-1360 (2018).

Yikai Wang and Yang-Tse Cheng, "A nanoindentation study of the viscoplastic behavior of pure lithium," Scr. Mater. 130, 191-195 (2017).

Reviewer 6:
The reviewer remarked that the current approach is focused on "ideal" materials without defects and grain boundary and noted that with over 70% of the project completed, no clear indication of key factors for design of interfaces was identified. The reviewer added that while electronic conductivity was experimentally shown to be an important factor, only highest occupied molecular orbit (HOMO)- and lowest unoccupied molecular orbit (LUMO)-like calculations are planned on ideal 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 found that all technical accomplishments are relevant and stay in line with scheduled milestones. The results obtained on Li mobility in solid-state Li nitrides using computational high-throughput ab-initio approach is very useful for designing novel Li-ion conductive solid-state electrolytes with targeted conductivity of approximately 10^{-3}S/cm. Also, the reviewer wrote, the continuum theory on dendrite propagation in the solid conductor helps evaluate different mechanisms of Li-metal penetration through the electrolyte volume. The reviewer concluded that this work demonstrated very good progress in addressing the key technical barriers of the Li-ion solid-state batteries.

Reviewer 2:
The reviewer remarked that Li-ion conducting nitrides exhibit better electrochemical stability as compared to oxide counterparts. The reviewer explained that a focus has been on the continuum-based modeling and identifying a criterion for Li dendrite penetration propensity and fracture modeling for crack propagation.

Reviewer 3:
The reviewer concluded that the program is on track and that milestones have been delivered on time.

Reviewer 4:
The reviewer commented that the individual approaches (ab-initio and continuum modeling) yield good progress, but they are not connected to each other. It was not clear to the reviewer if the good ionic conductors identified by ab initio in the first approach could have the interfacial properties modeled in the second

approach. In summary, the reviewer wrote, the results do not show a clear connection between the two approaches. The reviewer asked if the solid electrolytes selected from the ab-initio study are those analyzed in the second approach. The reviewer wanted to know what properties from the first group are input to the second group.

The reviewer found that, so far, progress of this project is in line with the milestones; however, it would be good to present performance indicators that demonstrate this progress. The reviewer stated that the study of the anionic frameworks is of great help for understanding transport of Li-ions and determines the low-barrier energy packings required for new solid-electrolyte materials. And the study of the imperfections on the surface of the Li-metal anode helps us to understand the redistribution and diffusion of the Li-ion; however, comparisons with experimental results are needed in order to validate the model. Finally, the reviewer remarked that a very negative point in this report is the lack of published papers.

Reviewer 5:
The reviewer stated it is unclear why Li-ion nitride was chosen for detailed modeling as high-conductivity solid electrolytes.

Reviewer 6:
After an extensive screening, it was not clear to the reviewer what experimentally validated materials were discovered to enable dendrite-free cycling of Li-metal. Noting that over 70% of the project is completed, the reviewer concluded that it is unlikely it will successfully produce new and experimentally validated models and criteria to identify promising solid-electrolyte materials that can prevent dendrite propagation in Li-metal.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer observed that the project team has been collaborating with LBNL as well as BNL and added that such a collaboration is very productive.

Reviewer 2:
The reviewer wrote that collaboration for computing resources— National Energy Research Scientific Computing Center (NERSC) at LBNL, ANL, and the Center for Functional Nanomaterials (CFN) at BNL— is duly noted.

Reviewer 3:
The reviewer stated that the program appears to be coordinated.

Reviewer 4:
The reviewer observed that the project team may explore collaboration opportunities with people who have published papers on the mechanical behavior of Li and that is important for their validation and modeling efforts.

Reviewer 5:
The reviewer noted that the project uses computational resources from LBNL and other Laboratories, but added that no other collaborations are shown in the report.

Reviewer 6:
The reviewer commented that the project is performed within a single group without noticeable collaboration with other modeling or experimental projects within the same program.

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

Reviewer 1:

The reviewer explained that in the future the project team plans to focus on several key tasks, such as an assessment of the electronic conductivity of various solid-electrolyte materials and determination of different mechanical and compositional criteria for preventing the Li-metal propagation in the solid-state conductors. The reviewer found that the proposed future work is well planned, seems logical, and makes perfect sense.

Reviewer 2:

The reviewer stated the project clearly outlines the tasks concentrating on electronic-conductivity screening and assessing the effect of mechanics for the stability of the metal and solid-electrolyte interface.

Reviewer 3:

The reviewer said the proposed future research is well planned and targets critical challenges.

Reviewer 4:

In addition to the three tasks, the reviewer noted that the project team may add tasks on validation and testing of theoretical predictions by collaborating with experimentalists.

Reviewer 5:

The reviewer concluded that the plan is good but it misses connections between ab-initio screened materials for high conductivity and mechanical properties proposed to control dendrite growth. The reviewer explained that there are some particular challenges to developing a model of solid-state interfaces for the protection and use of Li-metal anodes. The electronic leakage toward the electrolyte and fractures caused by bulk stress fields are the problems that this team has to deal with.

Reviewer 6:

The reviewer remarked that the proposed research goals seem to be relevant on the surface: however, screening of the SSE electronic conductivity seems to be limited to the defect and grain-boundary free materials and, therefore, might not correlate with the failure of realistic materials and dendrite growth at the realistic interfaces.

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

Reviewer 1:

The reviewer affirmed that the project is highly relevant and directly supports the VTO goals. The reviewer elaborated that design of solid-state batteries with low price, high energy density, and excellent cyclability is the main VTO program objective, and the present project contributes much into achieving this challenging goal.

Reviewer 2:

The reviewer agreed that the project is very important to reaching DOE objectives of batteries with high energy density and extreme fast-charging capabilities.

Reviewer 3:

The reviewer wrote that the program can help to enable use of Li-metal electrodes, which would lead to much higher energy density storage.

Reviewer 4:

The reviewer concluded the project is aligned with the goal to advance solid-state battery technology.

Reviewer 5:
The reviewer said the goals are relevant to increasing Li-battery energy density.

Reviewer 6:
Yes, the reviewer stated, the project supports overall DOE objectives of addressing instabilities at the Li-metal surface.

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

Reviewer 1:
The reviewer concluded that the project team has sufficient financial, computational, and human resources to complete the project in a timely manner.

Reviewer 2:
The reviewer commented that the computational resources from DOE supercomputers are great for this team.

Reviewer 3:
The reviewer said the team has access to required computing resources.

Reviewer 4:
The reviewer noted that program milestones are being met and it appears that the resources are sufficient.

Reviewer 5:
The reviewer stated the team may add experimental resources for validation of model predictions.

Reviewer 6:
The reviewer remarked that the number of publications and progress is low for the project resources.

Presentation Number: bat374
Presentation Title: Stabilizing Cathode/Electrolyte Interface by New Electrolyte Design
Principal Investigator: John Zhang (Argonne National Laboratory)

Presenter
John Zhang, Argonne National Laboratory

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

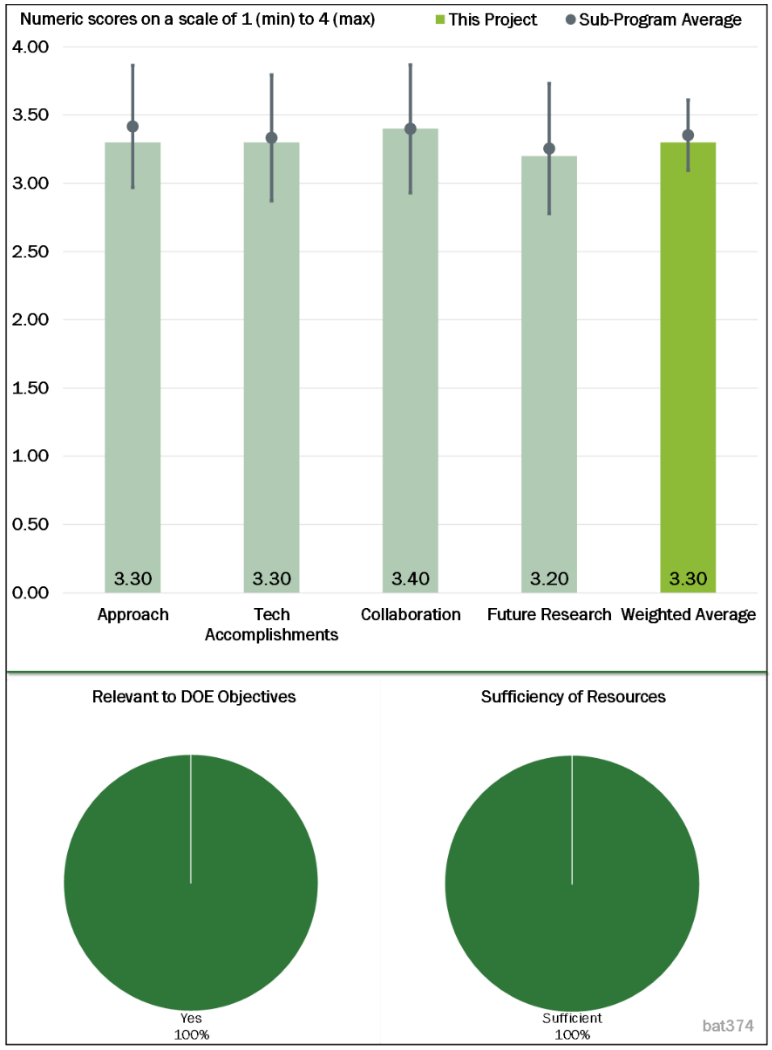

Figure 2-55 – Presentation Number: bat374 Presentation Title: Stabilizing Cathode/Electrolyte Interface by New Electrolyte Design Principal Investigator: John Zhang (Argonne National Laboratory)

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 stated that the approach seems good, adding that there is nice chemistry work. However, the reviewer wrote that MD simulation was lacking, and that stainless-steel contamination could be determined by looking for chromium (Cr) or vanadium (V) in system.

Reviewer 2:
The reviewer remarked that, in general, the approach is good as it potentially allows for the drop-in solutions for the industry. Since this is new project, the reviewer suggested it might be a good time to consider objectives that, if met, offer practical solutions. For example, the reviewer proposed first identifying the cathode compositions that offer the highest energy densities at the industry acceptable voltages (safety) and then investigating new electrolyte solutions to improve interface stability and cell's longevity. The reviewer wrote that the concern is that going to high voltages (please define) might be a logical path, but it might not be practical for many reasons for EV applications.

Reviewer 3:
The reviewer stated that high-energy cathodes require new, improved electrolytes, and this project is very important to figure out what is necessary from the electrolyte. The reviewer hoped to see some new ideas next year. The reviewer noted that fluorinated solvents and lithium bis(fluorosulfonyl)imide (LiFSI) have been around awhile, pointing out that, in fact, industry is already using LiFSI and the corrosion issues are well known.

Remarking that low-cost halide-free synthesis of LiFSI sounds interesting, the reviewer would like to have heard more about plans on this.

Reviewer 4:
The reviewer replied that this project discusses the use of ionic electrolytes with high-voltage cathodes, but added that the rationale for ionic liquids is not clear. The reviewer asked if there are no other organic electrolytes that cannot perform at these potentials.

Reviewer 5:
The reviewer explained that the technical approaches addressed new electrolyte design to attack the instability of high-voltage cathode and electrolyte. While finding this approach interesting, the reviewer remarked that, historically, the approach of using ionic liquid as electrolyte for Li-ion has achieved limited success, and it is unclear if the current approach in this project will be effective or not. Furthermore, the reviewer said it is unclear if the ionic electrolyte being studied is cost effective or not.

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 there is excellent work on identifying and addressing challenges associated with the use of the new materials. The reviewer said it will be interesting to see if there is a dependency of the transition-metal dissolution as a function of composition (Ni-content) versus the standard electrolyte used today. Provided industry is shifting to using high-Ni materials, the reviewer added that the use of new electrolytes proposed by the project team might be limited (the team found Ni as highly soluble).

Reviewer 2:
The reviewer wrote that chemistry progress seemed good but added that MD simulation needs to be revaluated to get meaningful information out of the simulation.

Reviewer 3:
Noting that this project just started in October, the reviewer thought the progress to date is adequate.

The reviewer hoped the project team is brainstorming some new ideas and chemistries, adding that five molarity (5M) LiFSI does not seem like a commercially relevant solution.

The reviewer was glad to see the issue of separator wetting being addressed.

Reviewer 4:
The reviewer stated that preliminary results of this project have showed some promising impact of high salt concentration. The reviewer was unsure if the compatibility of the designed electrolytes is compatible with both the anode and cathode at relatively higher temperatures. In addition, the reviewer was unsure if the designed electrolyte can work in a voltage range higher than 4.3V for cycle testing.

Reviewer 5:
The reviewer observed that this project is mostly looking at screening available ionic liquids and their utility with high-voltage cathodes. Noting that compatibility of such electrolytes with other components in battery electrodes has been investigated, the reviewer said there should be some rational selection of these compounds.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer found a good combination of people and analytical techniques, adding that the team has access to pouch cells, which is important for electrolyte development.

Reviewer 2:
The reviewer suggested the project team talk to the team associated with BAT252 and BAT253 on TM dissolution results.

Reviewer 3:
While the collaboration across the project team members seems good, it was unclear to the reviewer what the contribution from each project team member is.

Reviewer 4:
The reviewer said the collaboration seemed okay but suggested DFT calculations to predict binding energies and MD if the project team want to do lots of atoms. The reviewer said the project team should think about what information it wants out of the simulations.

Reviewer 5:
The reviewer was unclear who is doing what in terms of contributions. The reviewer remarked that in order to assess true collaboration, it is important to identify contributions of each of the partners.

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

Reviewer 1:
The reviewer found that all proposed tasks are well thought out and are relevant and could be easily amended to the modified objectives.

Reviewer 2:
The reviewer stated that the proposed future research is reasonable. The reviewer hopes to see some research on the cyclability of Li-ion cell with the designed electrolyte at higher voltage (greater than 4.3V)

Reviewer 3:
The reviewer responded that future works seemed good but suggested the team rely on DFT more than MD.

Reviewer 4:
The reviewer wrote that the "Future Work" section was kind of sparse and needs new ideas and new approaches. The reviewer recommended taking the time to get project team together and brainstorming new approaches and using Daniel Abraham's FOM approach to increase the dataset from which to draw conclusions and ideas.

Reviewer 5:
The reviewer found that the proposed research seems to be somewhat weak. The reviewer wrote that proposed studies include adding Li salts into ionic liquid and investigating their use with high-voltage cathodes. The reviewer said there should be a more rational approach to electrolyte formulations and/or through high throughput screening, adding that it is not clear what could be learn from such a combination.

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

Reviewer 1:
Responding that electrolytes are critical to enable new high-energy cathode materials, this reviewer thought they are underrepresented in the research funding. The reviewer added that enabling these materials is necessary for DOE to meet vehicle technology targets for energy storage

Reviewer 2:
The reviewer found great relevance to the DOE objective of improving battery technology.

Reviewer 3:
Noting that high-voltage cathodes are very important for high-energy-density battery systems, the reviewer remarked that in that regard, the electrolyte systems need to be designed and evaluated for such electrode systems.

Reviewer 4:
The reviewer commented that the project is very important for enabling new generations of cathode materials and suggested that the team might consider using compositions with higher Ni content for studies versus 532 used now.

Reviewer 5:
The reviewer replied that the design of a new electrolyte to stabilize the interface of electrode and electrolyte may support the DOE objectives on a high-energy 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 indicated the resources seems good.

Reviewer 2:
The reviewer replied that the resources assigned to this project seems reasonable.

Reviewer 3:
The reviewer stated that the resources are sufficient.

Reviewer 4:
This reviewer thinks resources are okay but suggested the project team get input from outside its organization.

Reviewer 5:
The reviewer suggested crosstalk with other PIs.

Presentation Number: bat377
Presentation Title: Lithium-Ion Recycling Center Overview
Principal Investigator: Jeff Spangenberger (Argonne National Laboratory)

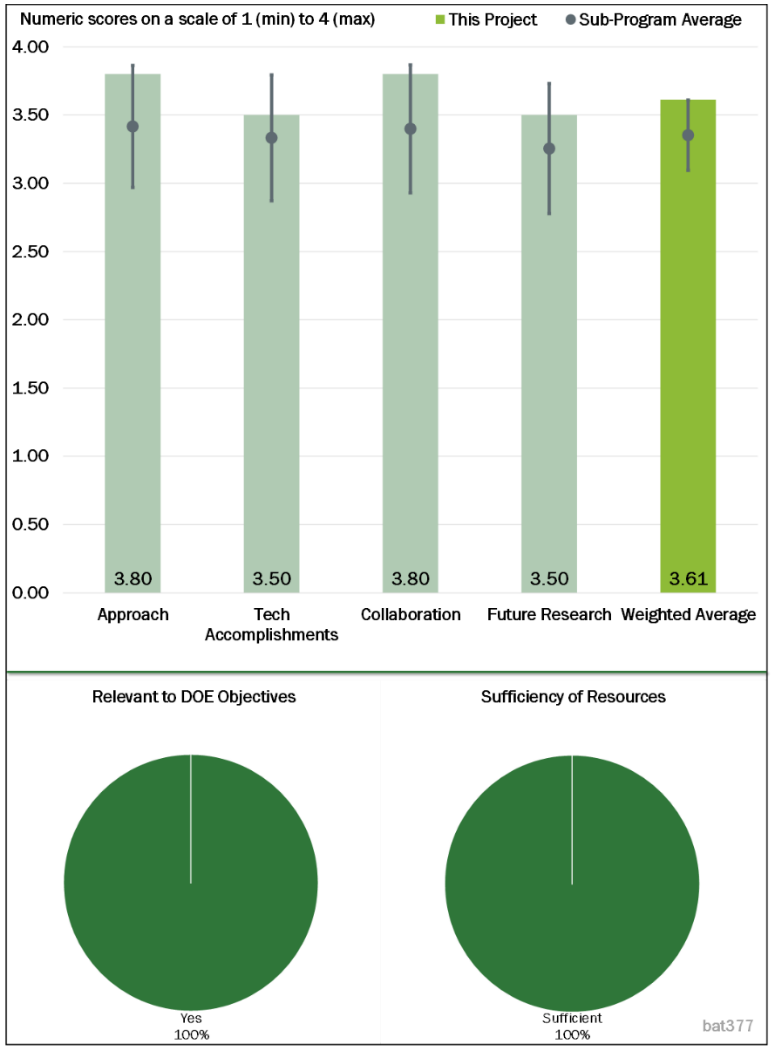

Figure 2-56 – Presentation Number: bat377 Presentation Title: Lithium-Ion Recycling Center Overview Principal Investigator: Jeff Spangenberger (Argonne National Laboratory)

Presenter
Jeff Spangenberger and Linda Gaines, 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:
This reviewer rated the project and the presentation as outstanding because the reasons for the need of a recycling projected were clearly outlined and presented, the supporting teams of this ReCell project were identified and their level of expertise in their contributing roles is excellent, and the appropriate near-term recycle candidate chemistries were identified. The reviewer added that the appropriate aspects of recycling concerns were clearly identified and summarized in preparation for the more detailed explanation of each area, and finally, the design and modeling efforts needed to support recycling were incorporated as part of the mission statement.

Reviewer 2:
According to the reviewer, the project is well designed to use modeling and analysis to guide the cathode materials recycling, other components recycling and cell design.

Reviewer 3:
The reviewer replied that the project is well designed and feasible based on the mission list on Slide 11 of the presentation. The reviewer elaborated that the overview identified the challenges and barriers that each project area would address, as well as the potential impact on the topic in general.

Reviewer 4:
The reviewer explained that the recycling center has four focus research areas—including Direct Cathode-to-Cathode Recycling, Other Materials Separation, Design for Recycle, and Modeling and Analysis for Recycling— that are well organized and covered all the components of current commercial batteries. The reviewer elaborated that the materials to be recycled include electrode powders, such as 10% chemically

delithiated NMC-111, lithium manganese oxide (LMO), and graphite, among others. Standard Operating Procedures (SOPs) will be used for the analysis among the four focus areas, which is good for comparison and evaluation.

The reviewer remarked it is good to perform quantitative analysis of the costs for recycling, elaborating that the costs of recycling should be compared with those of raw materials and the recycling percentage of materials should be provided.

Reviewer 5:

The reviewer commented that the project touches upon most of the important reasons to recycle. However, it missed the one built around reducing emissions of toxic materials to the environment, and in the same way, reducing the impact on human health, which should be of primary concern. The reviewer observed that the project design is very broad, including many aspects, technical challenges and solutions, and engages a broad collaboration. The reviewers were only provided some historical data on the cobalt market and one graph modeling the future to 70 years ahead without any comment.

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:

This reviewer rated the technical accomplishments and progress as outstanding because this Recycling ReCell is a very recent addition to DOE as a key enabler for a low-cost Li-ion battery; reaching the appropriate mission statement and identifying the appropriate team members and their contributions were completed, which was a difficult task; and setting up realistic goals for both the battery chemistries and the recycling processes that are to be evaluated was not an easy task, but was reached and are very appropriate.

Reviewer 2:

The reviewer explained that in the last year, the following was achieved: Through thermal treatment, binder was removed without significantly altering the initial electrochemical performance; hydrothermal delamination of graphite anodes was achieved while the optimization of the cathode-electrode delamination is still going on; the project team also developed an updated version of EverBatt that is now available for download; and finally, a methodology was established to obtain grain orientation from cathode samples via electron backscatter diffraction.

Reviewer 3:

The reviewer replied that the project covers a large diversity of technical methods and concepts but added that there are still points that could be clarified better. The reviewer noted that, currently, the cost of recycling is 5-15 % of battery cost but inquired about the scale. Currently, only a few percent of Li-ion batteries are recycled. The reviewer wanted to know how the effect of scale will alter this cost. Recycling reduces all emissions and energy use. Including graphs, the reviewer stated that these data are based on energy mix but wondered from which year and how those figures will evolve. The reviewer also asked whether the batteries are produced from recycled materials as safe as those produced from fresh materials; what the battery identification (ID) concept (e.g., containing data on chemistry, best recycling process, etc.) is, and what the recycling-related standardization issues and logistics are. The reviewer concluded that a robust recycling process is needed that works for all Li-ion battery chemistries and asked if it is not better to apply pre-sorting to direct different chemistries to the processes that are optimized for given formulation.

Reviewer 4:

The reviewer remarked that some technical accomplishments are not clearly justified by the cost analysis. For example, hydrothermal delamination of graphite anodes is likely to be a high-cost process yielding low-value product.

Reviewer 5:

The reviewer commented that the technical accomplishments and progress listed help to move forward the work being done, but the performance indicators were not clearly defined. Noting that this is a new project, the reviewer said how progress is being measured and what it is being measured against should be covered in more depth in future presentations.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

This reviewer rated the collaboration and coordination as excellent because the expertise and availability of the experimental equipment of the labs involved was fully utilized. So, the people and equipment needed to do the evaluation for the specific aspects are in place and this allows for a high level of efficiency and competence and the universities involved were noted for having programs, people, and a desire that was already linked with this technology development.

Reviewer 2:

The reviewer remarked that the collaborators list is impressive.

Reviewer 3:

The reviewer stated that the teams are well integrated and coordinated.

Reviewer 4:

The reviewer affirmed that the collaboration and coordination across the project team appears to be very good.

Reviewer 5:

The reviewer explained that the project was performed through the collaboration with ANL, NREL, ORNL, the University of California at San Diego (UCSD), WPI, and Michigan Technological University (MTU). The reviewer added that the team is well organized.

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

Reviewer 1:

This reviewer rated the proposed future research as excellent because the starting point of this recycling project is for recycling spent **cells** (NOT the entire battery) and this keeps the focus appropriately narrow; the narrow initial focus is on current and near-term chemistries, but the future goals address new and promising chemistries; direct recycling appears to offer the highest potential for cell-material cost reduction and the future work pushes for recycling projects that focus on this direction; and the

effort is initially doing demonstration projects using recycled material from these projects in cells, and, if successful, a demonstration of a continuous process are very appropriate future goals.

The reviewer added one comment on future work: The initial recycling Slides 7-10 indicates a starting point **of spent cells**. However, much of the cost associated with recycling vehicle batteries, to get to a cell, is the dismantling of the battery. Generally, in the recycling process, the entire battery is shredded to get to the materials. It was not clear to the reviewer that this cost is included in the cost analysis. The reviewer thought that the future work should include looking at how the cell materials will be recovered if the source stream is an entire module or battery rather than just a single cell.

Reviewer 2:

The reviewer remarked that this future plan is critical. Projects need to be evaluated for technical and economic viability and a down-select process is needed. The reviewer added that many ongoing processes are clearly not cost effective.

Reviewer 3:

The reviewer stated that the research team has planned their future work in a logical manner to meet the goal of the project. The reviewer elaborated that battery pre-treatment will be established to enable direct recycling and maximum material recovery. The EverBatt and the Libra models will also be improved. Batteries made from recycled materials in real applications and a continuous battery recycling line will be demonstrated in the future work.

Reviewer 4:

The reviewer replied that plans for future works are covering almost all relevant fields. The reviewer added, however, that safety of the batteries fabricated with recycled materials and environmental protection during the recycling logistics and processes should be included.

Reviewer 5:

The reviewer responded that future work is laid out in a logical manner and the challenges and barriers were defined. The reviewer added, however, that the decision points were not defined (or at least were not explored during the presentation).

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

Reviewer 1:

The reviewer commented that the recycling of batteries is very important for sustainability and to secure availability of raw materials. The reviewer elaborated that direct recycling can most efficiently recover the remaining value of the EOL batteries and hydro- and pyro-metallurgical processes are capable of coping with more non-homogeneous feedstock to recover the valuable materials. The reviewer concluded that all those strongly contribute to DOE objectives.

Reviewer 2:

The reviewer affirmed that this project is relevant as it has the strong potential to reduce **overall** battery cost by 10% or more. Additionally, the reviewer said, by recycling batteries in the United States, more valuable materials are retained in the United States that are not easily obtained. This project supports that material retention.

Reviewer 3:

The reviewer explained that this project is aimed at decreasing the cost of recycling Li-ion batteries to ensure future supplies of critical materials and decreased energy usage compared to raw material production. The reviewer added that it aligns well with DOE objectives to make the United States energy independent.

Reviewer 4:

The reviewer responded yes because the suite of projects under the ReCell umbrella are targeting DOE's objectives by trying to find ways to directly recycle materials that could lead to a lower cost battery if technologies and processes developed prove to be successful in real-world applications.

Reviewer 5:

The reviewer replied that the project is focusing on making recycling profitable, elaborating that all the targets and designs fit into the big picture for cost reduction. In particular, the reviewer said, it is important to recycle some elements such as Co and Ni, which are rare in the resources of the United States. The reviewer concluded that this project supports the overall DOE objectives to enable lower cost Li-ion batteries.

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

Reviewer 1:
The reviewer judged all the synthesis, characterization, and data resources for this project are sufficient.

Reviewer 2:
The reviewer responded that the resources are sufficient to achieve the stated milestones in a timely fashion.

Reviewer 3:
The reviewer stated the resources available to the project seem to be sufficient to run it.

Reviewer 4:
The reviewer remarked that the resources are sufficient for this project since the scope is reasonably narrow. The reviewer added, however, that the proposed future work can significantly expand the scope and more resources will be needed.

Reviewer 5:
The reviewer commented that specific milestones were not clearly defined; however, it appears that ReCell has enough National Laboratories and DOE support to make progress on the goals by the end of the 3 years.

Presentation Number: bat379
Presentation Title: Direct Cathode-to-Cathode Efforts
Principal Investigator: John Vaughey (Argonne National Laboratory)

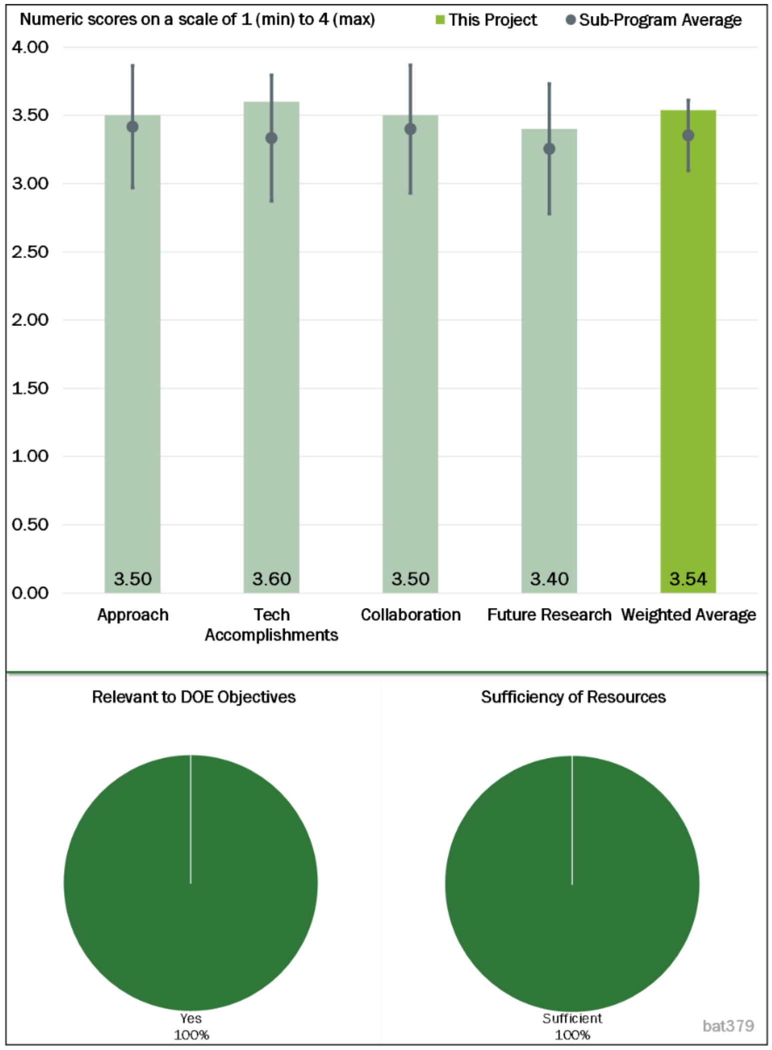

Figure 2-57 – Presentation Number: bat379 Presentation Title: Direct Cathode-to-Cathode Efforts Principal Investigator: John Vaughey (Argonne National Laboratory)

Presenter

John Vaughey, 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 battery recycling is critical to enable lower cost Li-ion batteries and also to ensure future supply of raw materials. The project is well designed, and the reviewer looks forward to seeing interesting results for upcoming year.

Reviewer 2:

Considering this beginning stage of this project, the reviewer liked how broad the approach is. The reviewer observed that the researchers are taking multiple paths toward addressing the various challenges surrounding battery recycling. The reviewer elaborated that recyclers will have to take as input batteries of many different and unknown chemistries, classify them by chemistry, remove inactive organic material, refresh the active material, and possibly upgrade the chemistry. The research plan is to look at each of these steps and, in most cases, pursue multiple paths to achieve the goals.

Reviewer 3:

The reviewer observed that recycling has become an important topic in the field and added that this direct cathode-to-cathode project works on almost all possible routes toward recycling the useful components in a battery. Multiple alternatives are used in the project, which can help mitigate the risk of project failure. Most approaches used are appropriate.

Reviewer 4:

The reviewer responded that the approaches are feasible to achieve the objectives of the project.

Reviewer 5:

The reviewer noted that various techniques have been explored for the initial separation of battery cathodes, binder removal, and cathode re-lithiation. The reviewer added that although technical methods have been explored, optimizing costs has not yet been demonstrated.

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 praised the technical accomplishments so far as excellent. The reviewer noted a few examples of initial success such as the chemical re-lithiation approach. The reviewer elaborated that if the PIs can better understand how each battery component fails and then design methods to recycle, that would be helpful. For example, cathode materials can fail due to many reasons, and the critical analysis of the failure modes can provide insight into developing recycling methods.

Reviewer 2:

The reviewer explained that the team has elaborated and carried out various strategies to address the problem of the separation of battery cathodes, as well as chemical methods for binder removal and re-lithiation techniques. Noting that preliminary results show some promise for froth flotation, the reviewer added that magnetic separation of NMC cathodes seems more difficult. Similar variability on the degree of success is observed for binder removal and cathode re-lithiation. The reviewer commented that the positive aspects are the exploration of a wide range of alternatives for these separations. Although the cost is not yet a significant variable, optimizing the technical separation seems to be a good goal for this stage. The reviewer suggested that perhaps an analysis of the minimum technical requirements in the desired product would be a good starting point to accept or reject techniques.

Reviewer 3:

The reviewer stated that the project has shown significant progress over a short period of time.

The reviewer wondered whether there is pH or collector dependency on Li contents cathode separation using the froth flotation method. Noting that fatty acid and hydroxamate effectively collect NMC-based cathode while magnetic fields have low efficiency, the reviewer asked if it is possible to place multiple recycling conditions in one stream, for example, froth flotation followed by magnetic field or vice versa. The reviewer asked the team to please comment on capacity increase of pristine NMC-111 full-cell cycle in Slide 12.

Reviewer 4:

The reviewer stated that the team has established the Center's mission but added it would be better if numerical targets (e.g., recovery cost versus the cost of raw material production) were included in the mission.

Reviewer 5:

Given that the project only started in October, the reviewer commented that expectations are modest. The reviewer noted that it looks like there is a feasible path toward separating LFP from other types of battery chemistries by simply relying on the hydrophobicity of the particles. However, the reviewer elaborated, it seems like the path to separating out NCA is still an issue. The magnetic work seems promising for its capability of separating LMO and NMC. The reviewer remarked that the progress slide was a bit confusing, though. It is clear from the data that lower magnetic flux is more effective at separating the two materials, and the improvement is monotonic with decreasing flux density. The reviewer also remarked that the researchers did not explain why even lower fluxes were not attempted. The reviewer concluded that results for binder burnout and re-lithiation are promising.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer noted that this project is part of a larger effort by multiple institutions and PIs.

Reviewer 2:
The reviewer commented that the project team has a very complementary set of expertise and is under the leadership of a well-known battery scientist and engineer.

Reviewer 3:
The reviewer stated that this project involves multiple PIs from a variety of National Laboratories and universities.

Reviewer 4:
The reviewer stated that the project team shares consistent materials and methods that provide comparable results among project team members. However, the reviewer added that it is too early to evaluate collaboration and coordination.

Reviewer 5:
The reviewer pointed out that there are quite a few different organizations involved in this project. However, the reviewer remarked that it appears that everyone is "doing their own thing," so the reviewer is unable to determine to what extent there is actual collaboration for any single project. Nevertheless, the reviewer said, coordination seems to be good.

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

Reviewer 1:
The reviewer said it was a well-thought plan.

Reviewer 2:
The reviewer stated that future plans are well addressed, noting new baseline cathode powders with higher amounts of de-lithiation and commercially relevant powders, re-lithiation, and controlling impurities, etc. The reviewer asked the project team to explore SOC (or Li contents) of dead batteries, particle distribution, and blending of different cathode powders (NMC-LMO, NMC-NCA, etc.). By doing so, the reviewer said the program will address more relevant Li contents and cathode materials for recycling.

Reviewer 3:
The reviewer replied the proposed future research is reasonable.

Reviewer 4:
The reviewer responded that the future research plan is clear for the most part. The reviewer encouraged the PIs to develop a strong materials-characterization program that can directly compare the recycled materials with the pristine materials. For layered materials, it is recommended that the characterization should be beyond the regular XRD that uses only the 003/104 peak ratio.

Reviewer 5:
The reviewer remarked that the large number of approaches reduces the risk that none of the approaches works. The reviewer hoped that there is some consideration of a down-selection process to put resources behind the most promising approaches and dropping the least promising approaches. The reviewer did not see

any attempt or plan to look at what the cost of these processes will be. For instance, binder removal seems to work best with slower burnout rates, but that will increase the time and cost of the recycling process.

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

Reviewer 1:
The reviewer declared, yes, recycling is definitely an important topic, adding that the technology may lead to overall lower battery price in the future.

Reviewer 2:
The reviewer stated that this project supports overall DOE objectives of recycling battery materials.

Reviewer 3:
The reviewer remarked that the overall DOE objectives are to reduce the cost of battery materials and minimize the environmental impacts of the battery lifecycle, adding that this project directly addresses those goals.

Reviewer 4:
The reviewer replied that lowering overall battery costs is important to adopt of EVs and that success of ReCell program supports the DOE objective since the cost to recycle is 5%-15% of battery cost.

Reviewer 5:
The reviewer responded that decreasing the cost of recycling Li-ion batteries has strategic value for further battery development, especially given the high cost of Co and Li.

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 entire team represents one of the best combinations of personnel, expertise, and facilities to secure the potential success of the project.

Reviewer 2:
The reviewer said it seems there are substantial resources for this project.

Reviewer 3:
The reviewer replied that resources are adequate to achieve the goals of this project.

Reviewer 4:
The reviewer said resource allocation is reasonable.

Reviewer 5:
The reviewer responded that resources are sufficient.

Presentation Number: bat380
Presentation Title: Other Materials Separation
Principal Investigator: Kris Pupek (Argonne National Laboratory)

Presenter

Kris Pupek, 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.

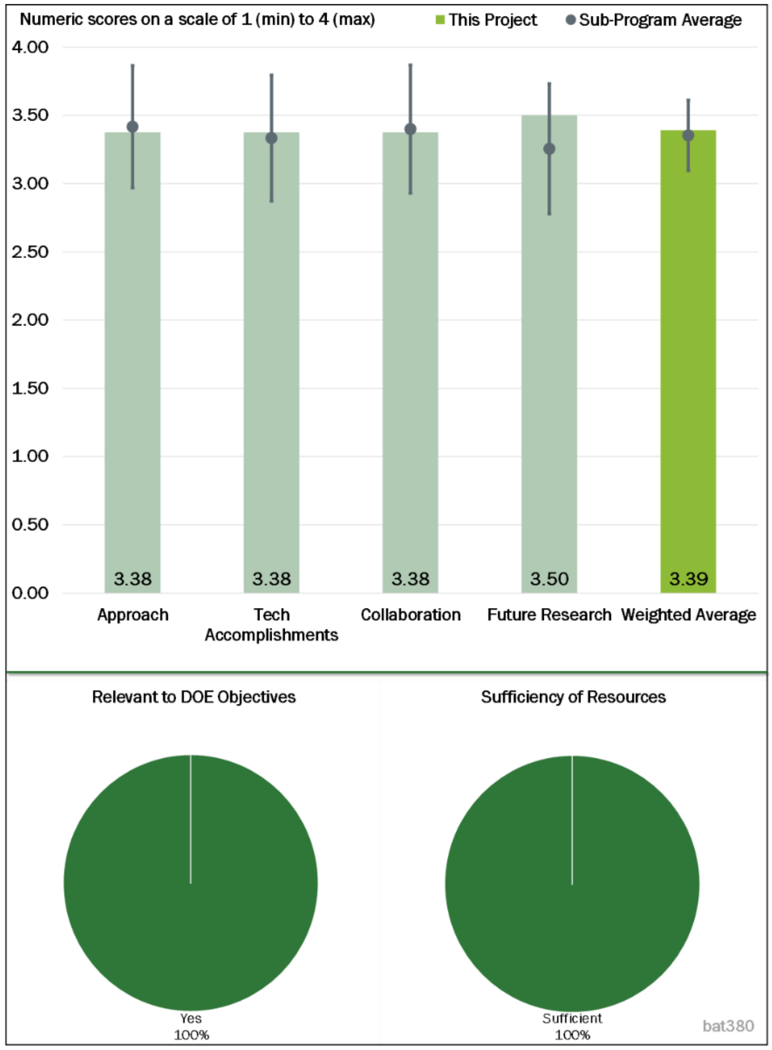

Figure 2-58 – Presentation Number: bat380 Presentation Title: Other Materials Separation Principal Investigator: Kris Pupek (Argonne National Laboratory)

Reviewer 1:

The reviewer stated that the project is well designed and feasible, elaborating that to maximize the potential of the recycling process, the investigators have studied all the materials that can be recovered and reused in commercial batteries. The reviewer added that the electrolyte-component recovery, anode-cathode separation, and hydrothermal delamination of electrodes are being performed. The recycled products facilitate a profitable recycling industry. The reviewer noted that the anode, cathode, and electrolytes of batteries will be recycled and said that it is good to rank the significance, value, and profit of recycling processes among these components. Also, the reviewer said the cost analysis should also consider the environmental impact of the wastes generated during recycling.

Reviewer 2:

The reviewer commented that the project team has developed multiple approaches for the electrolyte component recovery, anode-cathode separation, and delamination of electrodes. These are important steps for the recovery of Li-ion batteries.

Reviewer 3:

The reviewer found the collection of approaches in this project to be much more disparate than other recycling projects and added that it is not clear why these elements of recovery were chosen.

Reviewer 4:

The reviewer remarked that the researchers need to develop and down-select more effective anode-cathode separation methods. Additionally, the anode delamination process needs to be reevaluated using a cost model.

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 great progress for the first year.

Reviewer 2:

The reviewer responded that electrolyte recovery progress is satisfactory so far. Remarking that it is understandable that the project team is pursuing solvent extraction before supercritical carbon dioxide plus solvent extraction, the reviewer hoped, given the comparison table on Slide 6, they will pursue this in the future. The reviewer also stated that the anode-cathode separation work has revealed some major issues with dealing with shredded and unsorted cell waste in that there is significant contamination with small pieces of aluminum and copper. Given this fact, the reviewer thought that the project team should focus efforts on being able to remove this contamination from the feedstock. The hydrothermal delamination may be a more appropriate approach if this contamination cannot be resolved.

Reviewer 3:

The reviewer noted that different ways for electrolyte-component recovery were compared. In the solvent-extraction method, the reviewer explained that acetonitrile, dimethylformamide (DMF), tetrahydrofuran (THF) and diethyl carbonate (DEC) were chosen to extract the electrolyte from commercial battery electrodes. The reviewer elaborated that the extracted and recrystallized electrolyte was analyzed by nuclear magnetic resonance (NMR) and GC-MS. Recovered salts were evaluated with full-cell electrochemical tests. Additionally, the reviewer explained that black mass from shredded, unsorted EOL Li -on cells was analyzed after the anode and cathode separation using various methods. The separation quickly approaches 100% through magnetic separation using neodymium-based magnets. Delamination of the anode and cathode was investigated with the hydrothermal method.

Reviewer 4:

The reviewer stated that many experiments are still using very small amounts of samples and impractical long-time hydrothermal treatment. The reviewer suggested that more progress should be made to show how this process scales.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer responded that the project teams is well coordinated.

Reviewer 2:

The reviewer noted that ANL, NREL, ORNL, UCSD, WPI, and MTU work together on this project. The reviewer added that the project team is well organized.

Reviewer 3:

The reviewer said this project involves multiple partners from both National Laboratories and universities.

Reviewer 4:

Noting that a number of different institutions are involved, the reviewer did not see any coordination in their activities.

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 replied that the proposed research is reasonable and feasible.

Reviewer 2:
The reviewer thought the items listed in the future work are appropriate, but that more separation methods need to be tested.

Reviewer 3:
Based on the progress made so far, the reviewer explained that other methods will be investigated in the future work except for the solvent-extraction method used for electrolyte-component removal and recycling. Additionally, the reviewer noted that the impact of pre-processing method will be studied for the anode-cathode separation, and the feasibility of simple magnetic separation of additional cathode materials will be investigated. The process parameters for hydrothermal delamination of the anode and cathode will be optimized.

Reviewer 4:
The reviewer remarked that these process developments should be better guided by cost analysis.

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

Reviewer 1:
The reviewer stated that this project aims to decrease the cost of recycling Li-ion batteries to ensure a future supply of critical materials and decrease energy usage compared to raw material production. The reviewer concluded that it aligns well with DOE objectives to make the United States energy independent.

Reviewer 2:
The reviewer replied that this project addresses some of the issues facing battery recycling, which is a point of emphasis for DOE.

Reviewer 3:
The reviewer replied that this project will foster the development of cost-effective and environmentally sound processes to recycle Li-ion batteries, will reduce the cost of ownership, and help to drive down battery costs to meet DOE'S $80/kWh goal.

Reviewer 4:
The reviewer said that the efforts will help decrease the cost of the 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 found that all the synthesis and characterization resources for this project are adequate.

Reviewer 2:
The reviewer replied the resources are sufficient.

Reviewer 3:
The reviewer said the resources are sufficient.

Reviewer 4:

The reviewer remarked that the project budget indicated in this presentation reflects the budget for much more work than is included in this update. Therefore, this reviewer cannot really state whether or not the funding is sufficient, as the reviewer did not know whether the budget is for the work contained within this update.

Presentation Number: bat381
Presentation Title: Design For Recycling
Principal Investigator: Jianlin Li (Oak Ridge National Laboratory)

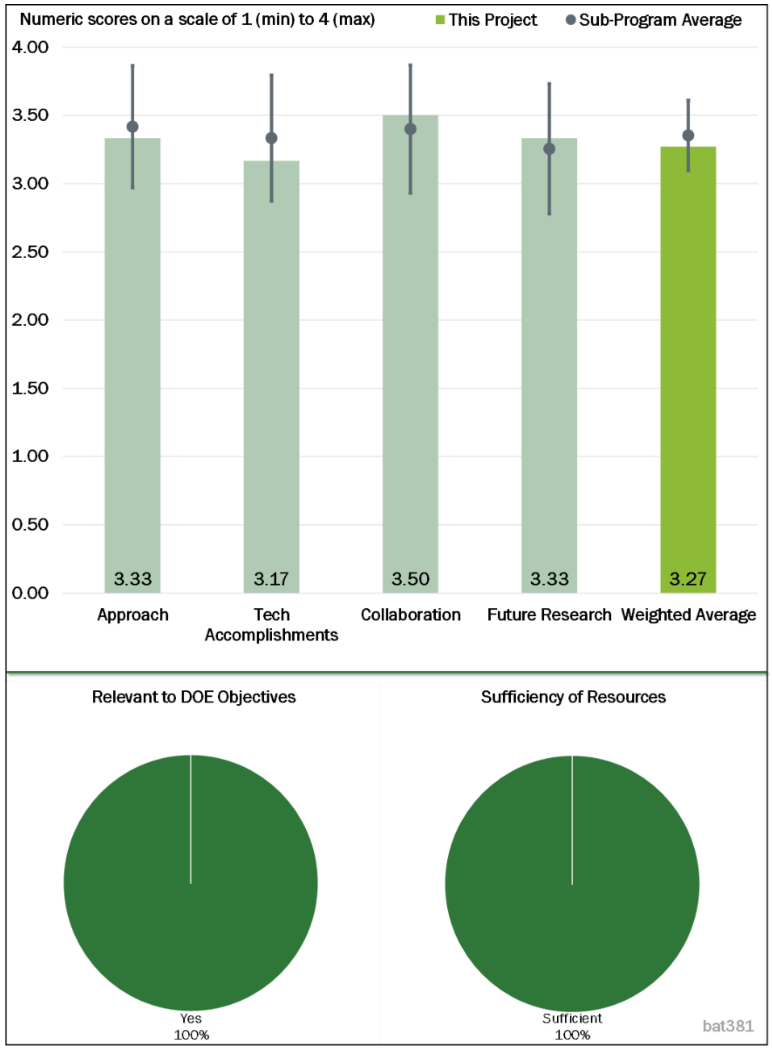

Figure 2-59 – Presentation Number: bat381 Presentation Title: Design For Recycling Principal Investigator: Jianlin Li (Oak Ridge National Laboratory)

Presenter

Jianlin Li, 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 praised the approach of looking at flow-through cells as an excellent idea.

Reviewer 2:

The reviewer explained that this project aims to develop new designs that will trade minimal loss in energy-density performance for the ability to use inexpensive recycling processes and make the batteries marketable, adding that the pouch cells and cylindrical cells will be designed. The reviewer also noted that this “Design for Recycling” project lies in one of the focus research areas in the Recycling Center. The reviewer recommended establishing the correlation of the designed cell configuration with the recycling processes. In other words, the reviewer said, please clarify how the new design of batteries will make the recycling process easier and reduce the cost of recycling.

Reviewer 3:

Stating that the project is feasible, the reviewer added that it was not always clear during the presentation what technical barriers needed to be addressed. In addition, the reviewer said, design for recycling may take a different form in the manufacturing space and could center around disassembly of a pack or module or cell. The reviewer suggested that a little more discussion on how (if successful) this process will impact and benefit battery manufacturing would be helpful in seeing a larger picture.

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 explained that the NMC-622 (3 mAh/cm^2) cathode and the capacity-matched graphite anode have been successfully fabricated and cylindrical and prismatic cells with ports were designed and fabricated for cell rejuvenation. Significant efforts were paid to seal the assemblies and ports. The relation between flow and pressure in prismatic cells was investigated. The reviewer remarked that the results show that the cell pressure increased with an increase in the flow rate and initial compression. Velocity dependence on inlet size and applied pressure were further investigated. The reviewer indicated the results show that the velocity was slower at the center of the cell with large inlet size due to more liquid flows toward the sides. The flow patterns and pressure gradient were further simulated.

Reviewer 2:

The reviewer noted that for the flow-through separator, the separator is 10 μ and the electrodes are 50-100 μ. The reviewer asked why the flow is expected to take place in the separator when the separator porosity is not that much greater than the porosity of the electrodes.

If the main goal is to dissolve away the SEI, the reviewer stated that the team would want the flow to go through the anode. Noting that the anode platelets lie flat on the current collector, there is a very low in-plane tortuosity. Since the project team probably wants most of the flow to go through the anode, and since this is what will happen naturally, the reviewer asked why there is any thought about encouraging flow through the separator.

The reviewer also asked how much energy is required to push flow through the cell. The reviewer remarked that if the cost of that energy is too high, then the project will not work, and it would be good to find that out at the beginning.

The reviewer wondered what the appropriate solvent is and how much solvent will be needed. The reviewer similarly remarked that if the cost of that solvent is too high, then the project will not work, and it would be good to find that out at the beginning.

The reviewer also wondered how the used solvent will be disposed of. Once again, the reviewer remarked that if the cost of disposal is too high, then the project will not work, and it would be good to find that out at the beginning.

Reviewer 3:

The reviewer indicated that this project is new for FY 2019 and the performance indicators were not clearly defined. The reviewer stated that it is clear the cells have been built and work is being done to characterize the flow pattern and velocity of the "fluid." The reviewer said more work needs to be done on cell assembly. The reviewer added that performance indicators should be included in future presentations, especially if there are correlating tests being run on the cells.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer described as good the collection of collaborators.

Reviewer 2:

The reviewer noted that this project is performed by ANL, NREL, ORNL, UCSD, WPI, and MTU.

Reviewer 3:

The reviewer observed that Slide 2 lists partners for this project but added that the role these partners will play in the project was not clear. As an example, the reviewer noted, it is stated on Slide 14 that the cells will be evaluated for lifecycle benefit from electrolyte rejuvenation, and it would be helpful to know which laboratories would be doing this work (if not the same as the laboratories creating the rejuvenated cells).

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 general, the reviewer remarked, the proposed future research will be effective. As the project evolves, the reviewer added, decision points and the impact of barriers should be added to future presentations. The reviewer added that it would also be helpful to know what tests are going to be run as part of the evaluations and what performance guidelines will be used to determine if the rejuvenation is successful.

Reviewer 2:
The reviewer explained that the flow pressure in the as-assembled cylindrical cell, cycled cylindrical, and prismatic cells will be characterized in the future work. Effort will be made to further rejuvenate the cycled electrodes. The reviewer elaborated that the cycle life, which benefits from the electrolyte rejuvenation, will be evaluated. Cylindrical and prismatic cells in proposed cell designs will be assembled and cycled.

Reviewer 3:
The reviewer is not convinced that a lot of the "showstoppers" have been considered. For example, the reviewer noted, without an appropriate solvent, the whole project fails, but no solvent has yet been identified.

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

Reviewer 1:
If successful, the reviewer stated, the new design of the punch cell and cylindrical cell will trade minimal loss in energy-density performance for the ability to use the inexpensive recycling processes. The reviewer agreed that this project supports the overall DOE objectives on reduced cost, reduced primary material production, and minimized environmental impacts.

Reviewer 2:
Yes, the reviewer said, this project supports the overall DOE objectives of the ReCell Center. The reviewer elaborated that the project is targeting a way to design cells so that they can be rejuvenated and reused, which can lead to a reduction in raw-material usage, as well as processing and manufacturing costs. However, the reviewer suggested that a portion of the project should include how this rejuvenated cell can be integrated with the current battery-manufacturing process, as well as the cost of disposal associated with resulting "product" that comes from flushing the cell in order to determine if any savings can materialize in real-world operations.

Reviewer 3:
The reviewer remarked that rejuvenation is a mostly unexplored opportunity

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 the synthesis and characterization resources for this project are sufficient.

Reviewer 2:
The reviewer replied "Okay."

Reviewer 3:
Based on the presentation, the reviewer commented, other DOE National Laboratories, in addition to ORNL and ANL, are involved but their roles within the project are not clear.

Presentation Number: bat382
Presentation Title: Modeling and Analysis for Recycling
Principal Investigator: Qaing Dai (Argonne National Laboratory)

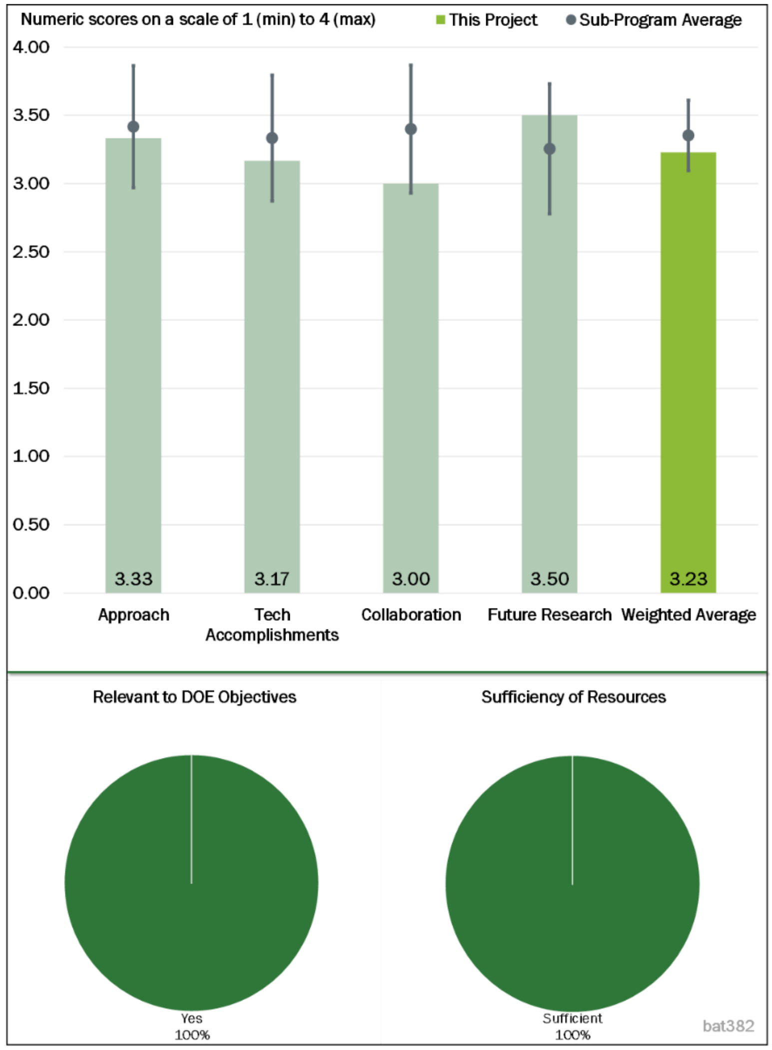

Figure 2-60 – Presentation Number: bat382 Presentation Title: Modeling and Analysis for Recycling Principal Investigator: Qaing Dai (Argonne National Laboratory)

Presenter
Qaing Dai, 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 modeling and supply-chain analysis tools are key to evaluating different process development.

Reviewer 2:
The reviewer explained that modeling and analysis will be used to direct researchers to the most efficient and economic potential recycling processes. The reviewer elaborated that diagnostics on aged materials, thermal analysis, techno-economic analysis (TEA) / lifecycle analysis (LCA) modeling (EverBatt), and supply-chain analysis will be carried out in this project. The reviewer said it would be good to use a large amount of data from experiments and literature to validate the model.

Reviewer 3:
The reviewer felt that this collection of topics adequately addresses technical barriers toward recycling but that it is unclear why these particular projects are grouped together.

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:
For the diagnostics on aged materials, the reviewer explained, the chemical signatures of a battery corresponding to its efficiency losses were identified by the electron back-scattering diffraction (EBSD). The reviewer stated that results matched the extent and type of degradation to target recycling methods. Additionally, existing NMC cathode compositions were thermally characterized, which helps to understand how the thermal signature of a battery changes from the beginning of life to the EOL. The reviewer said that

TEA-LCA modeling has estimated the cost and environmental impacts of recycling processes and the design-for-recycle strategies. Finally, the critical supply-chain questions for battery recycling were evaluated.

Reviewer 2:

So far, the reviewer remarked, EBSD has not been proven as a reliable tool for evaluating (either qualitatively or quantitatively) degradation mechanisms in battery electrodes. Micro-calorimetry has also not progressed far enough to evaluate its usefulness. The reviewer recognized this presentation only encompasses 6 months of work, however, so the reviewer hopes that things proceed further in the next year. The reviewer added that EverBatt appears to have quite quickly come to important conclusions on battery recycling.

Reviewer 3:

It seemed to the reviewer that diagnostics on aged materials and thermal analysis are not closely related to the modeling and supply-chain analysis tool development.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found that this project is well coordinated.

Reviewer 2:

The reviewer noted that this project was performed by ANL, NREL, ORNL, UCSD, WPI, and MTU.

Reviewer 3:

While there are a number of different contributors here, the reviewer did not see much in the way of coordination. Furthermore, the reviewer said, it was not quite clear how much coordination there could be, except for the two modeling and analysis projects.

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

Reviewer 1:

The reviewer replied that the future work is appropriate for this project. Given the early stage of this update, the reviewer added, future work encompasses much of the project plan.

Reviewer 2:

The reviewer wrote that future work will be focused on incorporation of the materials characterization parameters into EverBatt and efforts to continue to improve model usability. The reviewer elaborated that EBSD maps will be built for the cathode materials, which are recovered and treated by the different processes and that the relationship between performance and grain size and orientation will also be evaluated. In addition, heat generation at the beginning and the end of life will be evaluated using calorimetry to determine how the contaminants on cathode and anode affect the performance of the cells. The reviewer said it is interesting to evaluate the investment decisions for recycling and to analyze the material supply risk.

Reviewer 3:

The reviewer remarked that the correlation between first two efforts and modeling tool development needs to be further clarified.

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

Reviewer 1:

The reviewer stated that this project is aimed to decrease the cost of recycling Li-ion batteries to ensure future supply of critical materials and decrease energy usage compared to raw material production and added that it aligns well with DOE objectives to make the United States energy independent.

Reviewer 2:

The reviewer responded that modeling and analysis results will guide researchers to determine the most efficient and economic recycling processes. The reviewer added that the project supports the overall DOE objectives of enabling lower cost Li-ion batteries

Reviewer 3:

The reviewer said this project addresses various aspects of battery recycling and seeks to reduce risk and uncertainty in the battery-recycling process.

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

Reviewer 1:

The reviewer concluded the resources for the project are sufficient.

Reviewer 2:

The reviewer responded that all the characterization and data resources for this project are sufficient.

Reviewer 3:

The reviewer noted that the budget listed in the slides is for a set of projects much greater than the subset of project reviewed here. Therefore, this reviewer cannot evaluate if the resources are sufficient for the projects that are being evaluated here.

Presentation Number: bat383
Presentation Title: Understanding the Impact of Local Heterogeneities During Fast Charge
Principal Investigator: Eric Dufek (Idaho National Laboratory)

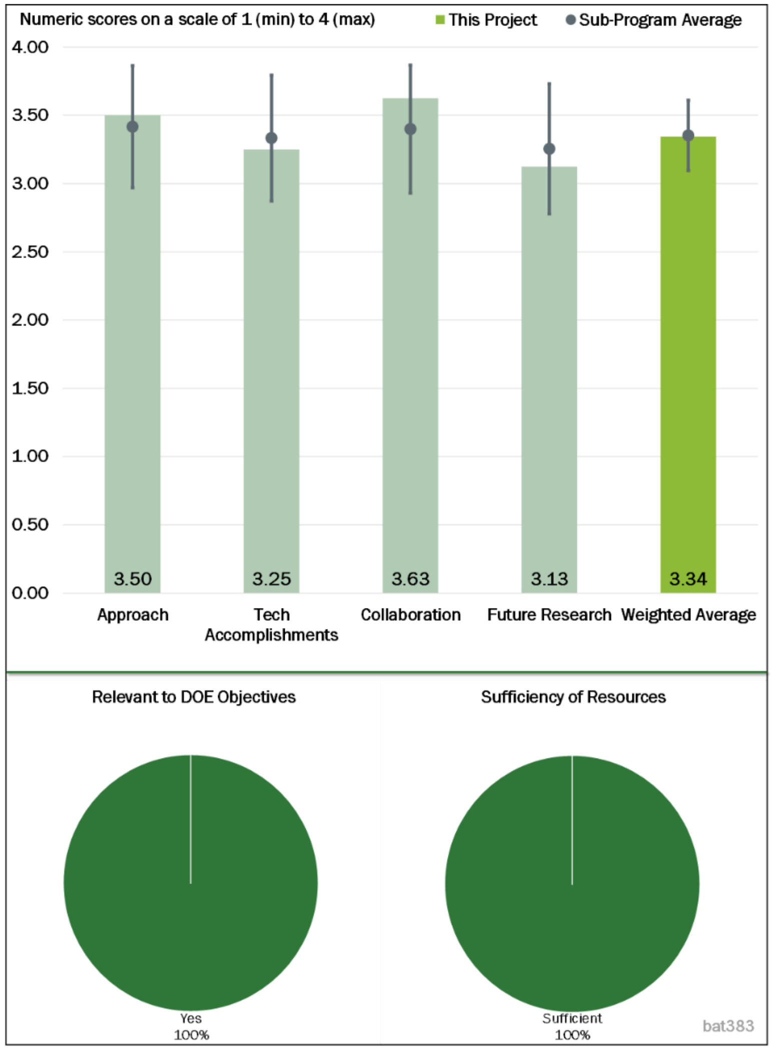

Figure 2-61 – Presentation Number: bat383 Presentation Title: Understanding the Impact of Local Heterogeneities During Fast Charge Principal Investigator: Eric Dufek (Idaho National Laboratory)

Presenter

Kandler Smith, National Renewable Energy 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 observed a good focus with balance of very fundamental study along with d more applied study.

Reviewer 2:

The reviewer appreciated the simulation and modeling approach being undertaken. The reviewer believed that both the atomic level and continuum scale level are important during this process.

Reviewer 3:

The reviewer remarked that quantifying electrode heterogeneity during rapid charging by using multiple tools such as modeling and tomography is innovative and complements the experimental data. The reviewer added that this approach will predict and guide electrode design to enable fast charging.

Reviewer 4:

The reviewer replied that the researchers methodologically identified and explained the patterns of Li plating and that they utilized experiments and modeling to quantify their findings and guide designs.

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 established milestones are accomplished as planned and that there is properly allocated sufficient time to carry out the unfinished projects in the third and fourth quarters. The reviewer also noted the project team had developed atomistic models to establish relationships between different variables affecting the fast-charging process and used electrochemical models to quantify heterogeneity influences on localized onset of Li plating to provide a detail understanding of length scales.

Reviewer 2:

The reviewer remarked technical accomplishments and progress are on the increasing diffusion coefficient of Li within graphite as a function of rate. Noting that there are several reports of high-diffusion coefficients for graphite in the literature, the reviewer is curious about how the understanding here agrees or disagrees with existing work. For example, K. Persson has also used nudged-elastic band (NEB) to calculate diffusion barriers within graphite (DOI 10.1021/jz100188d). She found very high diffusion coefficients. The reviewer wondered if it could also be that Li diffusion is slow at slow rates, rather than high at high rates. That is, perhaps the phenomenon could be viewed from the other direction. The reviewer elaborated that a concrete question is how the barriers calculated here translate to actual diffusion coefficients. The reviewer acknowledged there is not a precise calculation, but an order of magnitude can be determined.

On the continuum modeling, the reviewer said it is nice to see the model being used to consider effects both in two-dimensional (2-D) at the edges, as well as model studies of different shapes and sizes of particles.

Reviewer 3:

The reviewer remarked that findings regarding dual-coated electrode and impact on onset of plating as well as edge-effect prediction seem like particularly valuable accomplishments. The reviewer would like to better understand any related outcomes with actual cells and comparison of the model with actuals.

Reviewer 4:

The reviewer found intriguing the development of an atomistic model to understand improved diffusivity in the graphite. The reviewer wondered whether excess electrons during initial lithiation come from carbon additives in negative formulation or not. The reviewer stated that utilizing computerized tomography (CT) imaging of graphite grade used in the program enables the best particle-design strategy for fast charging, and it could be useful input to graphite manufacture. The reviewer said it might be useful if similar method can be applied to positive electrodes.

The reviewer also remarked that proposing the best electrode structure is valuable information, but it is also critical to check the feasibility of making such an electrode in the real world. For example, the reviewer noted, it is difficult to make an ellipsoid-shaped graphite particle aligned along the electrolyte transport direction since orientation of graphite particle can be altered during the calendering process.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer replied that researchers collaborated across multiple National Laboratories to complete the project. The reviewer elaborated that each laboratory has its unique capabilities and the researchers explored thoroughly and coordinated very well.

Reviewer 2:

The reviewer said that teamwork is obvious and praised it as great.

Reviewer 3:

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

Reviewer 4:

The reviewer responded that the project appears to show good collaboration across the project team, and the involvement of the specific university partners looks excellent and is described usefully.

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 plan with a further focus on predictions of aging effects from fast charging should be very valuable.

Reviewer 2:
The reviewer concluded that the future research plan seems to be reasonable, adding that it is important to keep improving fidelity of multiscale modeling.

Reviewer 3:
The reviewer remarked that atomic-scale modeling had concrete proposals for future work, and this is good. However, the reviewer suggested that this proposal should be revisited based on existing work in the literature and how this somewhat controversial proposal fits in.

Reviewer 4:
The reviewer said proposed future research identified critical gaps in the projects and developed a clear roadmap to address the gaps. The reviewer added that investigating at the sub-particle level provides more insight, and the development of predictive modeling helps the vast majority of the user community. However, the reviewer remarked that the continuum-modeling proposal is too soft and should be fleshed out to directly the support ongoing experimental activities.

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

Reviewer 1:
The reviewer replied that the DOE objective of fast charging under 15 minutes is addressed thoroughly in this project. Additionally, the project addresses the critical parameters and gaps controls the fast charging process. The reviewer concluded that the team has clearly outlined the current issue and a path forward to achieve the DOE objective.

Reviewer 2:
The reviewer stated that fast charging is very important to make EVs competitive with internal combustion engine (ICE) vehicles.

Reviewer 3:
The reviewer affirmed that the program will be able to help to achieve the DOE goal of lowering battery cost to less than $100/kWh.

Reviewer 4:
The reviewer said the project supports progress and understanding toward higher battery energy densities and/or higher charge rate capabilities for BEVs.

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 while the resources are very significant and appear to be at least sufficient (or beyond), the output and progress so far, and as planned, seem to be of significant and of corresponding value.

Reviewer 2:

The reviewer replied that collaborating across different laboratories and utilizing in-house expertise, both tangible and intangible resources are sufficient for completion of the project on time.

Reviewer 3:

The reviewer stated that resources seem sufficient to support the current level of research.

Reviewer 4:

The reviewer responded that resources are sufficient.

Presentation Number: bat386
Presentation Title: Extreme Fast Charge Cell Evaluation of Lithium-Ion (XCEL) Batteries
Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

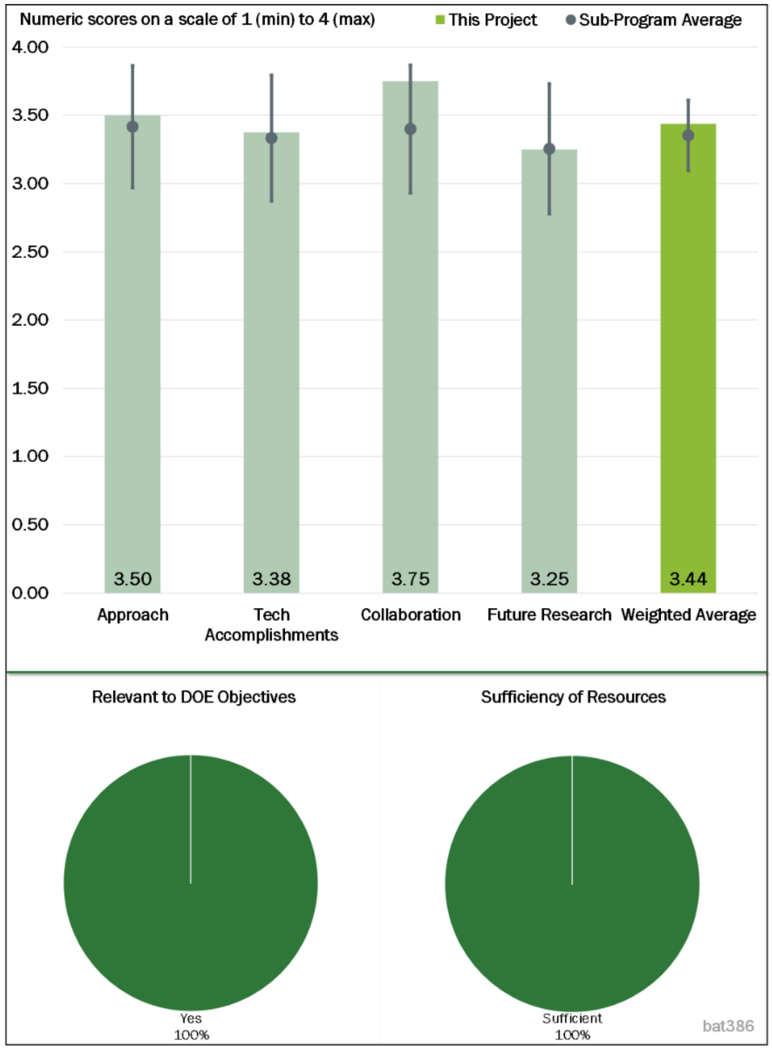

Figure 2-62 – Presentation Number: bat386 Presentation Title: Extreme Fast Charge Cell Evaluation of Lithium-Ion (XCEL) Batteries Principal Investigator: Venkat Srinivasan (Argonne National Laboratory)

Presenter
Venkat Srinivasan, 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 the combination of all sub-projects in this activity is well focused on this important area and is providing timely and valuable findings.

Reviewer 2:
The reviewer said that several different National Laboratories presented their work on fast charging process/methods.

Reviewer 3:
The reviewer remarked the team approach and tools being used are the right ones. The more detailed approach could be redirected to result in a higher impact for industry. The reviewer will detail these in the Results and Accomplishments question.

Reviewer 4:
The reviewer commented the questions that the program tries to answer would be a solid foundation for solving problems related to fast-charging.

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 the researchers clearly presented the impacts of the anode, cathode, and electrolyte on fast-charging process. Their findings were measured against performance indicators clearly. The reviewer noted that technical accomplishments and progress were mapped to the established milestones.

Reviewer 2:
The reviewer said the program accomplished significantly over a short period of time. The reviewer looks forward to seeing more progress next year. More emphasis on positive materials might be required in addition to addressing problems in graphite anode.

Reviewer 3:
The reviewer commented the accomplishments of the combination of projects to date is excellent and appears to be proceeding well. The reviewer said one missing element which should be included sooner rather than later is work to understand the impact of cell compression/pressure and/or cell expansion forces, as dependency on these simple mechanical parameters may significantly influence the specific outcome of many of the studies, and is important as we consider real-world solutions to fast charge issues.

Reviewer 4:
The reviewer commented the presented results are a good start, but it is time to conduct more precise experiments.

For example, blindly charging at 6C is a less than optimal experiment. Perhaps the approach should be, what is the maximum charging rate with lithium (Li) plating as a function of electrode physical properties (loading, N:P [negative to positive ratio], etc.)? The reviewer said that is a much more meaningful result than charging and then opening a cell to see if there is massive plating or not.

The reviewer pointed out that the state of charge (SOC) window is critical. The highest likelihood for plating comes at higher SOCs. Maybe it would make sense to split up the charging to everything that happens up to 50% and then what can happen after that. The reviewer thought that this could perhaps be “sold” as developing a charging strategy that is similar in timespan to filling the tank of an internal combustion engine (ICE) power vehicle. Maximize the amount of energy that could be charged in 5 minutes or something similar. The reviewer noted that this initial charging period is the most important to the customer, and we need to maximize miles per minute of charging.

The reviewer said that SiO_x at levels less than 10 weight % in the electrode is a very important path to simultaneous energy density and fast charging goals. There are cells going into cars that will be sold at the end of this year and beginning of next year that have these levels of SiO_x. The reviewer said, clearly, some level of silicon (Si) in some forms is ready for commercialization, and the DOE funded research should be ahead of the curve and not following.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said that this is a collaborative effort across multiple National Laboratories using their unique expertise, nicely done

Reviewer 2:
The reviewer commented the program uses a well-coordinated collaborative structure.

Reviewer 3:
The reviewer remarked the effort for collaboration and team work comes across.

Reviewer 4:
The reviewer observed, generally, collaboration appears to be and probably must be working well and must be being well coordinated in order to achieve the overall combination of accomplishments and progress to date. However, commented this reviewer, a better illustration of the specific contributions of the university partners may help illuminate the extent of collaboration across 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 indicated the project identified future research in a methodological way. Most of the work on fast-charging is focused at least now at the 25° Celsius (C) temperature. It will be beneficial if the researchers consider, extreme heterogeneous weather conditions due to different latitudes in fast-charging.

Reviewer 2:

The reviewer said correlating plated Li and capacity fading using X-ray technique was very intriguing and provides valuable information even in the same cells where manufacturing variation comes into play. The reviewer said identifying maximum charging rate to buffer manufacturing imperfections during electrode/cell preparation would be an interesting topic.

Reviewer 3:

The reviewer characterized propose future research as generally excellent, and to please refer to specific comments for each sub-project in this area. Again, the plan to include greater work on compression/pressure and/or cell expansion force sooner rather than later may be one critical partial path adjustment.

Reviewer 4:

The reviewer referenced prior comments, and remarked this is an applied problem and the work needs to reflect that. The reviewer said it is fine to focus on understanding, but in situ and operando are great but only if done under realistic conditions (i.e., on the edge of where plating begins rather than dramatic plating over the whole area).

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

Reviewer 1:

The reviewer pointed out that fast charging is critically important for electric vehicles (EVs).

Reviewer 2:

The reviewer said this project completely supports the DOE objectives and initiatives. There are several gaps exists in the fast-charging process and researchers have identified the gaps and developed a proper road map to address it.

Reviewer 3:

The reviewer said that the program is well-aligned with DOE goals.

Reviewer 4:

The reviewer remarked the project supports progress and understanding towards higher battery energy densities, and/or higher charge rate capabilities for battery electric vehicles (BEV's).

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 the resources for the stated milestones of the specific sub-projects in this area may be sufficient, but a greater number of projects and funding would be beneficial to further accelerate understanding and development in this critical overall area of fast-charging.

Reviewer 2:
The reviewer said that sufficient time and resources were allocated to each project associated in the fast-charging process.

Reviewer 3:
The reviewer said that resources are sufficient, and the reviewer is looking forward to seeing the results next year.

Reviewer 4:
The reviewer remarked the resources are adequate for the scope of the project.

Presentation Number: bat387
Presentation Title: Silicon Electrolyte Interface Stabilization Update with Question and Answer Session
Principal Investigator: Anthony Burrell (National Renewable Energy Laboratory)

Presenter

Anthony Burrell, National Renewable Energy Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

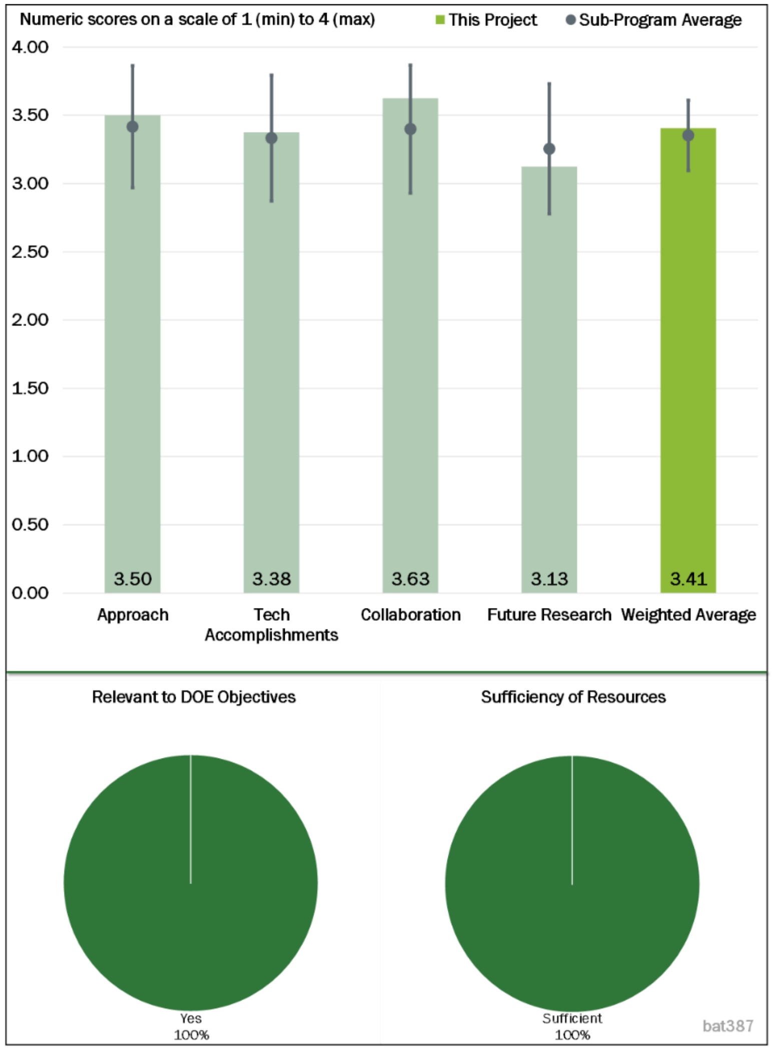

Figure 2-63 – Presentation Number: bat387 Presentation Title: Silicon Electrolyte Interface Stabilization Update with Question and Answer Session Principal Investigator: Anthony Burrell (National Renewable Energy Laboratory)

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:

This reviewer admits to rarely gives an outstanding rating—but this effort deserves it. Seek first to understand. That is what our National Laboratories should be doing. This is a very complicated system, and the reviewer appreciated the systematic effort by the team to decouple effects. The reviewer's only stated concern is that because results are very dependent upon the particular Si—that what you learn here will not matter for real world systems. However, you have to start somewhere.

Reviewer 2:

The reviewer characterized the project as a fundamental research based on great teamwork for better understanding the formation and evolution of the silicon electrolyte interface (SEI) layer on Si. Both theoretical and experimental methods were included in this work to prove and characterize the SEI layer compositions and its growth. The reviewer commented experimental findings were reconfirmed through cross checking using different analytical methods.

Reviewer 3:

The reviewer detailed that this collaborative project aims at acquiring a fundamental understanding of the formation, reaction, and stability of SEI layer on a Si anode. The team's choice of using SEI on Si wafers as a simplifying model platform for experiment study is reasonable and essential for achieving the targeted goal. It ensures the consistency in samples and reaction conditions and greatly facilitates detailed surface characterization. The reviewer said that the strong emphasis the team puts on the standardization of sample preparation and characterization protocols is highly commendable. This year the project focused on understanding the effect of the initial SiO_2 present on the Si surface on the subsequent evolution of SEI layer and its reaction with electrolyte. The reviewer remarked this is an important and technically relevant question as Si almost always has surface oxide on it. The approach the team took to characterize the SEI, electrolyte, and released gas species with a large array of techniques (X-ray photoelectron spectroscopy [XPS], Fourier transform infrared [FTIR], Raman, nuclear magnetic resonance [NMR], and GC-MS) is well-thought out and appropriate. The reviewer said that the preparation of model Li silicate samples with composition gradient through co-sputtering is interesting. The reviewer thinks some careful study should be done to confirm their composition and structure similarity to SEI from electrochemical reaction. In addition to surface chemistry characterization, transmission electron microscopy (TEM) study of the crystallinity and heterogeneity of surface SiO_2 after reaction with Li will provide useful complementary information. The reviewer said the combination of atomistic modeling and characterization to understand the SEI composition (Li-Si-O phase diagram) and the stabilizing effect of electrolyte additive (FEC) on SEI is excellent.

Reviewer 4:

The reviewer clarified the given rating for this question. If the goal is "Understand the fundamental chemistry and materials science of highly controlled Si-based samples in the presence of typical Li-ion electrolytes," the reviewer thinks the work would be "excellent" or "outstanding."

However, in this reviewer's view, getting Si particles or other shapes/forms to cycle in a liquid electrolyte with a CE and stable SEI is extremely unlikely. We can understand the fundamental science of what is happening, but the reviewer thinks a fundamentally different approach will be needed, such as encapsulation, so this reviewer is unconvinced the science done here will prove useful to developing solutions to the barriers.

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 the project is doing nice fundamental science work, and bringing true rigor to the subtle materials science and chemistry issues present in both the Si and the SEI. As the presentation says, when looking deep into the details here there is the "Bad and the Ugly," the reviewer pointed out that the chemistry is really complex and difficult for stability.

Reviewer 2:

The reviewer said simply making sure you characterize your materials before you start doing electrochemistry is a big accomplishment—thank you! The reviewer thinks the understanding the researchers have achieved on the role of SiO_2 is important and can help lead to solutions, which should be the ultimate intent.

The reviewer remarked the combination of experiments and calculations was done very well. The mobility of Li in Si and SiO_2 yielded good information. The reviewer thinks the combination of analytical techniques is key to figuring out the species and where they go, and it looks like the researchers have done a good job utilizing those techniques.

The reviewer was a little confused—Slide 2 says the project runs from October 2016 to September 2019, but the project is only 40% complete. How does that work?

Reviewer 3:

The reviewer said that rigorous analyses were carried out to figure out and ensure which composites are included during SEI layer formation and their behavior with the Si anodes. Additional information was provided such as how the SEI layer grows and what could impact its growth giving indication of possible solution to resolve the issue associated with SEI layers.

Reviewer 4:

The reviewer said that a main finding of the project is that Li silicates, the reaction products between SiO_2, Li and electron, are not stable and decompose in contact with electrolyte over cycling. Although the study does not suggest a beneficial role of SiO_2 on stabilizing SEI, the learning is meaningful and represents significant progress in the understanding of Si SEI. The reviewer said that it will be useful if the team could propose possible reactions between silicates and electrolytes and verify them with experiments in well-controlled environment.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

This is a big project and the reviewer thinks the results are impressive. The reviewer pointed out that could not have happened without good collaboration and coordination across the project team.

Reviewer 2:

The reviewer remarked the team made serious efforts to ensure effective collaboration between team members and well-executed coordination among various tasks, which can be challenging for such a large-scale project. The implementation of standardized sample preparation and experimental procedure is very helpful. The reviewer said the collaboration between modeling and characterization efforts and with the Silicon Deep Dive project is also productive and rewarding.

Reviewer 3:

The reviewer said that it appears the project is well-organized and integrated across many labs. Common samples and test fixtures are a best practice it appears the team is using.

Reviewer 4:

The reviewer pointed out that each team seemed to get their own work scope and targets to tackle the technical issues together. The reviewer said the speaker emphasized the frequent and thorough communications among research teams to plan and design the experiments for multiple characterization of the samples together leading to clear evidence of findings in 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 found that the topics appears good—especially looking at what happens when cycling is carried out. That is obviously critical for understanding in the battery context.

Reviewer 2:

The reviewer remarked based on the outcomes from this research, the project teams planned to identify solutions for stabilization of SEI layers. It would be great to team up with the battery industry to include recommended methods to keep the stabilized SEI layer through the usual manufacturing processes, such as cell formation processes.

Reviewer 3:

The reviewer remarked that the proposed future research is reasonable. Because the project finds SiO_2 not beneficial for stabilizing SEIs, the reviewer thinks one question worth further study is what we want to do to the surface oxide that always forms on Si. The reviewer wondered should we strip it before cycling or try to modify its properties with ways such as doping.

Reviewer 4:

The reviewer cannot tell how long this project will run if it ends in September 2019 but it still has 60% left. If it does have significantly more time or budget, the reviewer would like to see more specifics stated in the Future Work slide. These are general comments to continue doing what you are doing.

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

Reviewer 1:
The reviewer said this project is well-aligned with DOE objectives for an increase in energy density and a decrease in the cost of batteries.

Reviewer 2:
The reviewer pointed out that we need higher capacity cathodes and anodes to achieve DOE energy storage targets for automotive applications; Si is a big part of this roadmap. Efforts to make Si work and yield long cycle life are critical to hitting targets.

Reviewer 3:
The reviewer remarked the project is addressing DOE battery metrics.

Reviewer 4:
The reviewer remarked this project supports the overall DOE objectives by providing fundamental knowledge and support to address the key stability issue of the high-energy Si anode.

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 it seems like this is a large team with world-class capabilities. If this team cannot make progress on this problem, no one can. The reviewer inquired if the team is short of people that you cannot spend the funds. This is back to the issue with the project dates versus the fraction of the project complete.

Reviewer 2:
The reviewer pointed out that this is an expensive project, but the National Laboratories are doing detailed and high-quality scientific work.

Reviewer 3:
The reviewer said this project is for fundamental research requiring a lot of resources to achieve the milestones in a timely manner.

Reviewer 4:
The reviewer remarked the allocated resources (budget, personnel and equipment at multiple National Laboratories) are appropriate for the scope of the project.

Presentation Number: bat388
Presentation Title: Silicon Deep-Dive Update with Question and Answer Session
Principal Investigator: John Vaughey (Argonne National Laboratory)

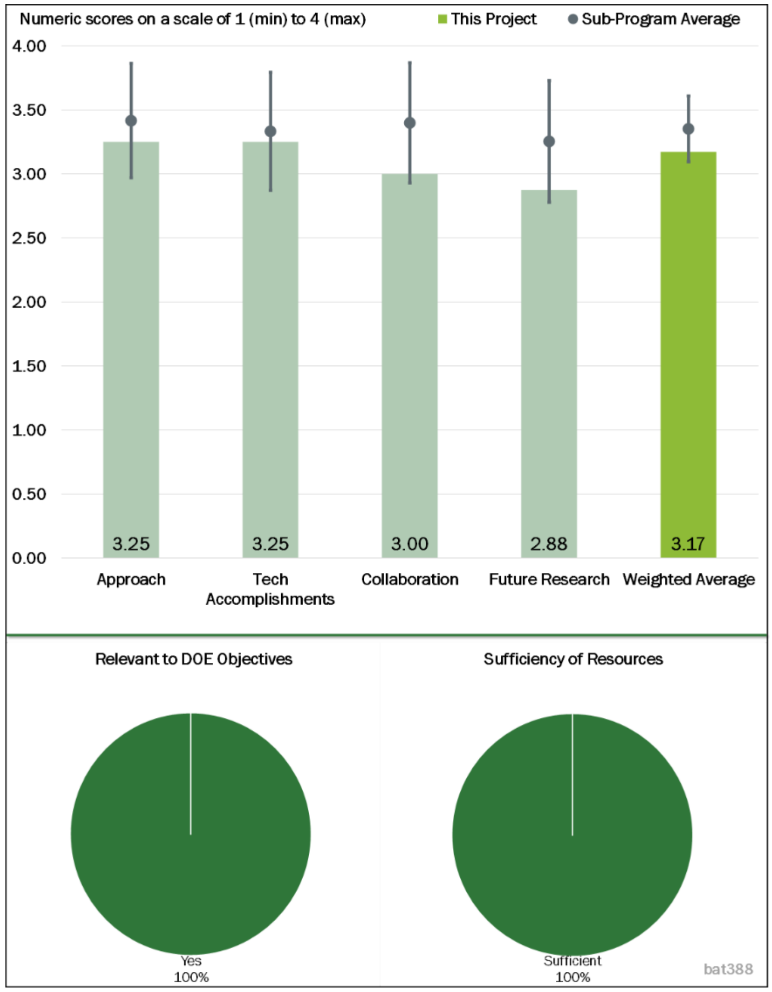

Figure 2-65 - Presentation Number: bat388 Presentation Title: Silicon Deep-Dive Update with Question and Answer Session Principal Investigator: John Vaughey (Argonne National Laboratory)

Presenter

John Vaughey, 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 pointed out that the Silicon Deep-Dive program is a multi-laboratory effort to address the key technical barriers faced by the successful incorporation of Si into the next-generation battery anode. The project attacks the stability problem of Si broadly from several different directions that complement each other, including the development of new coatings, binders, and concentrated electrolytes to stabilize SEIs and mechanical integrity. The reviewer said that this multi-pronged strategy is well-designed, synergistic, and in fact essential to meet the daunting commercial requirement placed on the Si anode. The reviewer noted that the project team also has the broad and complementary expertise in materials and electrolyte development, interface engineering, characterization and battery testing, which inspires a lot of confidence in the successful execution of the project.

Reviewer 2:

The reviewer said that most of the major cell components were verified for the Si-based anode life improvement. The reviewer pointed out that a wide range of materials were selected and examined using various analytical methods and verified by full cell cycling, giving direct information of the effect of each design change on the Si-anode based Li-ion battery life.

Reviewer 3:

The reviewer found it difficult to follow this presentation. Various strategies are being pursued—materials development, interfaces, evaluation—but it is hard to tell the significance of each of the individual efforts, and whether the overall project is meant to be exploratory, or to truly go after solving specific issues of silicon anodes. The reviewer did not see specific quantitative metrics (for example, as a cell level), so presumably the project is more exploratory.

Reviewer 4:

The reviewer remarked this project feels a little hit and miss. Some of the efforts are novel approaches with promising results. Others seem a little less relevant. The reviewer expressed appreciation for the many different approaches taken, and realize that some of them will not work. But, for example, the binder study only includes polyacrylic acid (PAA) and Li-PAA. The reviewer said that industry uses carboxymethyl cellulose (CMC)/ styrene-butadiene rubber (SBR)—and there are a lot of options for those materials. The reviewer said that it would be valuable to include more binders.

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 detailed that a range of the cell components from electrode active materials to electrolyte were screened and their main functionalities for cell life and performance improvement were examined with Si based anodes. The reviewer said the effects of the new materials were validated through both half and full cell tests providing direction for the choice of materials for Si-based anode research and development.

Reviewer 2:

The reviewer said that the project team has made impressive progress on multiple fronts this year. The stable Li-Mg-Si zintl coating is a very interesting discovery that looks really promising. The team also demonstrate surface functionalization of Si with epoxy to improve the adhesion to current collectors. The reviewer asked if these two approaches can be combined. The careful study on the effect of binder preparation on electrode slurry processing and performance is appreciated by the reviewer. The reviewer said the insight that PAA binds preferentially to Si and Li-PAA to graphite is an important one. The development of new concentrated electrolytes that significantly improve Si's cycling stability is another highlight of the technical achievements. The reviewer said that though each of these advances is significant by itself, the reviewer thinks it is important to explore how they can be integrated into the same cells to synergistically improve the stability of Si to the fullest degree.

The reviewer is a little confused by the finding that the capacity of graphite is largely inaccessible in Si-graphite (Gr) cell and most charges are stored in Si. The reviewer asked, if this is the case, why does the cell with only 15% Si and 73% graphite have almost identical capacity as the one with 70% Si after about 200 cycles.

Reviewer 3:

The reviewer said that the approaches presented all appear to make some improvement over a baseline, but often there are other factors that determine whether an approach is truly viable. The reviewer cited as an example, adding magnesium (Mg) salts appears to show some improvement on Si anode cycling, but there are likely side effects that are not mentioned. The reviewer remarked it is not clear the project is addressing all barriers.

Reviewer 4:

The reviewer said, again, this is hit and miss. The electrolyte work looks very promising, and really builds from the fundamental studies done by Burrell et al. But other areas are less productive and useful. The reviewer asked, for example, the Si-tin (Sn) composites showed that adding Sn helps, but the presenter only showed 20 cycles. The reviewer asked what's next for that project, and is this a viable solution.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer pointed out that this is a cross-laboratory collaborative project. Expertise from each National Laboratory enabled thorough investigation in potential materials for improvement of Si based anodes.

Reviewer 2:
The reviewer said that collaboration appears to be well organized among the team members.

Reviewer 3:
The reviewer remarked there is strong collaboration across the project team that effectively utilizes and integrates the wide-ranging expertise of team members in surface chemistry, materials synthesis, electrolyte development, and battery evaluation. The reviewer pointed out that the Deep-Dive team also demonstrated collaboration with the Silicon Electrolyte Interface Stability (SEISta) team to incorporate the fundamental insights (e.g., Li-Mg-Si surface coating stability) acquired by the latter into technical development.

Reviewer 4:
The reviewer felt like this was a report on 20 different projects instead of one cohesive 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 remarked right direction for the future research by figuring out the major mechanisms of the electrode structural change through advanced characterization techniques potentially providing information on further improvement of cell life and performance.

Reviewer 2:
The reviewer said the proposed research work is reasonable and consistent with the project goal. The proposed advanced characterization of electrode structure changes is important for obtaining a mechanistic understanding of various Si stabilization approaches. In addition to the investigation of individual elements, the reviewer said it is also important to evaluate whether the developed new coatings, surface functionalization, binders and electrolytes can come together to synergistically provide a path to meet the Office of Energy Efficiency and Renewable Energy, Vehicle Technologies Office (EERE VTO) goals.

Reviewer 3:
The reviewer said that the Future Work slide had several very broad statements to basically continue work already being done. The reviewer thinks it is time to rule out most of the team's approaches and focus on what is working the best or what techniques have the most promise to figure this out. Bring the team together.

Reviewer 4:
The reviewer said that future work again appears exploratory, with no quantitative metrics as a goal. Hence, it is not clear if all the DOE barriers will be truly addressed.

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

Reviewer 1:
The reviewer noted that we need higher capacity cathodes and anodes to achieve DOE's energy storage targets for automotive applications; Si is a big part of this roadmap. The reviewer said efforts to make Si work and yield long cycle life are critical to hitting targets.

Reviewer 2:
The reviewer pointed out that Si anodes address DOE goals.

Reviewer 3:
The reviewer remarked this project supports the overall DOE objectives by addressing the critical technical challenges faced by the stabilization of high-energy Si anodes.

Reviewer 4:

The reviewer said these research outcomes can impact DOE goals of cost reduction and life & performance improvement of the advanced energy storage systems.

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

Reviewer 1:

The reviewer said this is a big project, and it appears resources are sufficient.

Reviewer 2:

The reviewer found that the right teams with expertise are involved in the project and the entire project team seems to have enough resources to complete the next milestones in a timely manner.

Reviewer 3:

The reviewer said that the allocated resources (budget, personnel and facilities at multiple National Laboratories) are appropriate for the scope of the project.

Reviewer 4:

The reviewer said that the team would get more done working as a single team instead of a bunch of smaller projects.

Presentation Number: bat389
Presentation Title: Improving the Stability of Lithium Metal Anodes and Inorganic-Organic Solid Electrolytes
Principal Investigator: Nitash Balsara (Lawrence Berkeley National Laboratory)

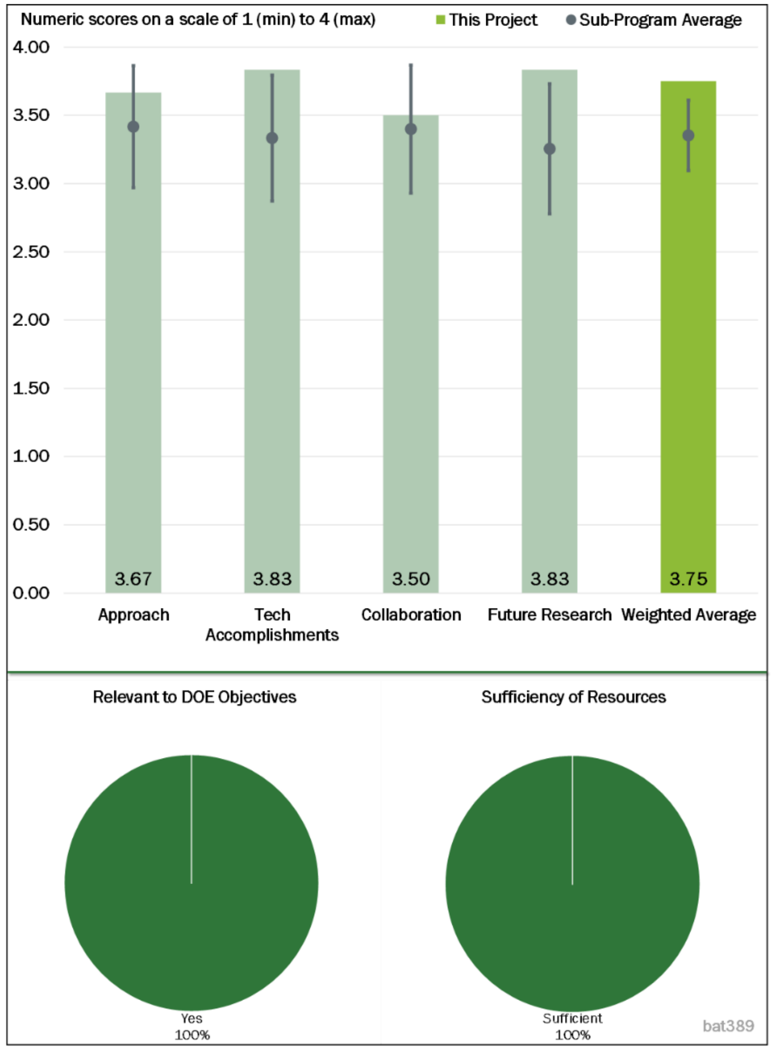

Figure 2-66 – Presentation Number: bat389 Presentation Title: Improving the Stability of Lithium Metal Anodes and Inorganic-Organic Solid Electrolytes Principal Investigator: Nitash Balsara (Lawrence Berkeley National Laboratory)

Presenter

Nitash Balsara, 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 said that a composite electrolyte is a good way to go for the achievement of Li-metal anodes in solid electrolytes. The project is well-designed and feasible.

Reviewer 2:

The reviewer said that the work approach is a very nice balance of synthesis of new materials, advanced characterization including microscopy and spectroscopy (e.g., NMR and impedance spectroscopy), and a reasonable theoretical component. The reviewer pointed out that by focusing the approach on a couple of key aspects of understanding the nature and dynamics of the solid-solid Li metal-solid polymer electrolyte interface, the project design is efficient and likely to produce the most significant results. Indeed, in the first half of the 1-year project, there have been few if any problems or limitations with the basic approach, and a series of significant results has been obtained in a short period of time. The reviewer said that the only "complaint" is that some initial full cell testing would have been helpful to include to get an early indication if Li-Li metal cycling really is a good model system for understanding the nature of the Li dendrite issue with polymeric solid-state electrolytes (SSEs) like the one developed in this project.

Reviewer 3:

The reviewer noted that the approach is to develop new ceramic-polymer composite electrolytes to enable Li-metal anodes, to identify failure modes at Li-metal anodes using synchrotron hard X-ray tomography, and to study the Li-metal/electrolyte interface by spectroscopy and impedance.

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 despite being started only a few months ago, the project has achieved several very significant milestones. Notably, the team synthesized and got initial materials (e.g., modulus) and electrochemical characterization data in symmetrical cells for a very interesting and promising hybrid organic-inorganic polymer electrolyte. The reviewer said that incorporating polyhedral oligomeric SilSesquioxane (POSS) as a mechanical block greatly improves the modulus while demonstrating reasonable ionic conductivity—which is notable because earlier block co-polymers (BCP) electrolytes had a much greater decrease in ionic conductivity when PS blocks where used to improve the mechanical properties. The reviewer said the team seems to have found a very interesting sweet spot in the trade-off space—and it is certainly worth exploring this promising material further to see if 1 mS/cm can be reached. But the team also completed some very nice work on mapping the electrochemical cell conditions that favor dendrites versus no dendrites and the role of the limiting current. The reviewer remarked this work very nicely illustrates why the higher modulus and higher limiting current (both the experimental value and the even higher theoretical value) of the new poly(ethylene oxide) (PEO)-POSS is likely to result in much higher current densities being possible without dendrite formation. Having the data and theory to explain the apparent advantages of PEO-POSS was very good work. Finally, per the reviewer, the discovery that Li-metal dissolves (or apparently dissolves) in polymer electrolyte is very exciting—and assuming it holds up in the scientific community after being published soon—this work could be the most important accomplishment of the project. The concept of Li as an electrode in the polymer electrolyte will certainly change how people think about designing a polymer electrolyte for Li-ion with or without Li-metal as the anode.

Reviewer 2:

The reviewer noted that this team demonstrated the conductivity was reduced by a factor of 2 while the modulus of PEO-POSS is 1,000,000 times larger than PEO. The decrease in conductivity is much less in PEO-POSS than SEO. The reviewer said that the POSS-PEO-POSS hybrid triblock electrolyte shows a higher limiting current compared to PS-PEO due to favorable transport properties, 12 mA/cm^2 versus 2 mA/cm^2.

Reviewer 3:

The reviewer commented that a very high critical current density of Li-Li cell has been achieved based on the composite electrolyte. The reviewer said it would be great if the full cell data tested at high current densities is also provided.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked the collaboration is great, given the resources of this project.

Reviewer 2:

The reviewer remarked Venkat Srinivasan (Argonne National Laboratory [ANL]) and Bryan McCloskey (University of California-Berkeley [UCB]/Lawrence Berkeley National Laboratory [LBNL]) are collaborators on this project.

Reviewer 3:

The reviewer acknowledged that it is hard to evaluate the level of collaboration in such a short project, but there are indicators that the collaboration is okay but could be better. For example, while there are clearly aspects of modeling in the dendrite work, this contribution does not show up (or has not yet) in the authors list on the papers just published or submitted. It does not mean that the collaboration is not happening, it just is not easy to see if it is. The reviewer commented that right now, it looks like most of the work is synthesis and characterization (mostly Balsara) with only a small (albeit important) modeling here or there to support it. The reviewer said there may not be much room for additional collaborations, but maybe there is.

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 it is really hard to see how the proposed work could be better—it seems to be exactly the right set of experiments to do next. Like the overall approach, the work outlined for the remainder of the project is well-balanced and very strategic. The reviewer said there is a nice mix of activities to demonstrate both performance (hopefully for the PEO-POSS electrolyte in a full cell with some Coulombic efficiency data) and the basic understanding that underlies that performance. Very nicely done.

Reviewer 2:

The reviewer detailed that the following tasks are proposed as future work: combining limiting current measurements and complete electrochemical characterization to determine current distribution during Li dendrite growth; compare experiments with calculations based on the full Newman model; working on methodologies to purify Li; study the cycling characteristics of purified Li electrodes; continue to work on polymer-based composites to reach the DOE target of 1 mS/cm (other transport properties really matter); determine the solubility limit of Li-metal in polymer electrolytes (single-phase and composites); determine the effect of salt concentration on the solubility limit of Li-metal in polymer electrolytes; obtain explicit signature of the free electron in Li/PEO and other electrolytes (electron paramagnetic resonance); and begin work on Li dendrite formation in full cells. The reviewer said that as mentioned during the presentation, purer Li will be provided by testing full cells. This seems like a good option. The reviewer pointed out that alternatively, one could sputter Li, but that can also have impurities if not done with due care.

Reviewer 3:

The reviewer said that the proposed research is reasonable and helps to achieve the objective of the project. It will be interesting to see the effect of Li-metal dissolution in PEO on the full cell performance.

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

Reviewer 1:

The reviewer said that the alignment between project objectives and DOE goals is very strong. If successful, the project will have significant impact on DOE’s ability to reach key milestones on their roadmap for energy storage—particularly for batteries with high capacity (Li-metal) and increased safety due to no flammable solvent and no dendrite formation.

Reviewer 2:

The reviewer pointed out that enabling a Li-metal anode will increase energy density and result in lower cost, based on $/Wh.

Reviewer 3:

The reviewer said that Li-metal battery can potentially offer 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 noted that this is a very short project with limited resources, but the approach has been very efficient and was created with a clear strategy. Thus, the project has a more than reasonable chance of achieving the stated milestones by the end of the project—but this reviewer emphasized that it still will be very impactful if it falls a little short of the 1 mS/cm performance goal for the hybrid polymeric electrolyte.

Reviewer 2:
The reviewer said that resources are sufficient to meet the project's goals.

Reviewer 3:
The reviewer remarked resources are sufficient.

Presentation Number: bat391
Presentation Title: Lithiation Method for High-Energy, Long-Life Lithium-Ion Battery (L3B)
Principal Investigator: Andrew Colclasure (National Renewable Energy Laboratory)

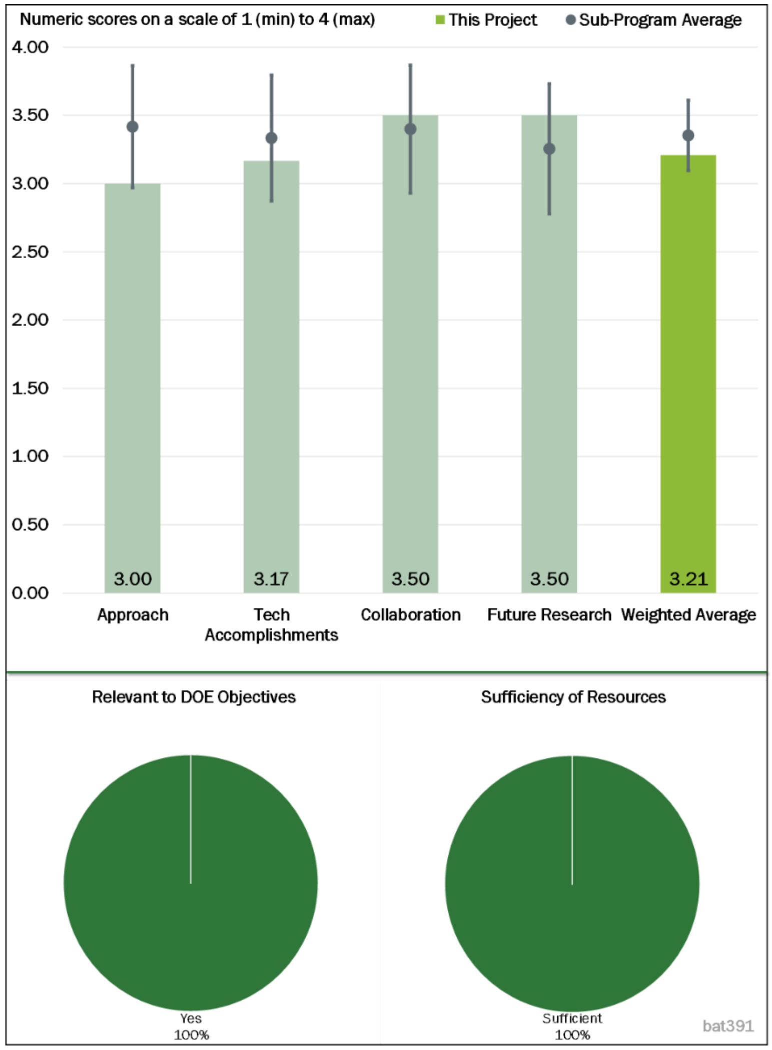

Figure 2-67 – Presentation Number: bat391 Presentation Title: Lithiation Method for High-Energy, Long-Life Lithium-Ion Battery (L3B) Principal Investigator: Andrew Colclasure (National Renewable Energy Laboratory)

Presenter

Andrew Colclasure, National Renewable Energy Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

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

Reviewer 1:

The reviewer pointed out that with passive control (merely a resistor), lithiation will happen slowly but all the way. This design may over-lithiate the cathode and cause irreversible decay. There lacks understanding on how fast Li-metal is consumed, and whether there is any remaining Li-metal after a few cycles. The reviewer said that the amount of Li-metal is not reported, and because Li metal is only at the side of the pouch cell, the uniformity of lithiation is of concern. The non-uniformity is studied, but not addressed.

Reviewer 2:

The reviewer detailed that this project is examining a Li-metal reservoir to extend the lifetime of Li-ion batteries. As Li is consumed by the SEI, Li^{+} is added to the electrolyte (from the Li-metal reservoir) to replenish the Li-ion inventory, thus restoring battery capacity. The reviewer said that a cell with an internal Li metal (Li^{+}) reservoir with passive control of Li-ion release was investigated. The method allows for both continuous and on-demand Li-ion release and it has minimal impact on the cell volume, mass and presumably cost (although a cost analysis has not yet been performed).

The reviewer noted that the principal investigator (PI) has used the method with a Si-graphite anode (with considerable capacity fade with cycling due to Li-ion consumption as the SEI layer ruptures and reforms) and with a graphite anode Si was chosen to accentuate and accelerate Li loss during cycling, i.e., only 50 cycles are needed to see capacity fade due to Li^{+} depletion.

Reviewer 3:

The reviewer remarked the approach to increase cycle life for batteries using Si anodes was partially addressed. This approach works only for few specific applications. Because along with capacity loss, impedance rise will equally limit battery life. Impedance rise is not addressed by this approach. The reviewer remarked the design is limited to small size of the cell. For large automotive cells, the location/design of re-lithiation system becomes complex using this approach. The reviewer said the robust control of the re-lithiation system is needed to prevent over lithiation that can lead to Li plating. This introduces reliability risks. The reviewer said the approach does not address loss of electrolyte during continued SEI formation, and it also does not address how changing Li concentration affects SEI quality.

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 project progress to the declared milestones was excellent. The team was able to demonstrate cell assembly successfully in a pouch cell, and results demonstrated successful re-lithiation of cell and extension of life. The reviewer remarked the models developed to control lithiation rate and prevent Li plating were significant developments.

Reviewer 2:

The reviewer remarked the PI has made nice progress on the project. All 2017 and 2018 milestones have been completed. 2019 milestones are on track for completion, and progress has been made over the past year. The reviewer noted that the concept was successfully tested on Si-graphite/ nickel manganese cobalt (NMC) and graphite/NMC pouch cells. The reviewer detailed that for an ANL-Cell Analysis, Modeling, and Prototyping (CAMP) Facility pouch cell (Si-GR anode and NMC532 cathode), the lifetime was extended by 200%, using multiple, triggered re-lithiations while room temperature cycling at C/3. For a baseline case, cells faded to 280 mAh after 60 cycles. With re-lithiation, the cells had a capacity of 280 mAh after 180 cycles.

Reviewer 3:

The reviewer is confused on the controlled release. On one hand it is claimed that no third terminal is required, on the other hand artificial start and stop of release is done, as shown in Slide 10.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said good collaboration with industry partners and ANL in cell build.

Reviewer 2:

The reviewer remarked the team has demonstrated active collaboration.

Reviewer 3:

The reviewer noted some collaboration with ANL, and that interactions with two companies (Coloumetrics and Nanograf) were minimal.

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 research is well planned, although alternative approaches could be added.

Reviewer 2:

The reviewer said that future work is reasonable and logically follows what has already been accomplished. The team focus on large capacity cells suitable for EV applications is appropriate. The reviewer remarked more work is needed on the placement of the Li reservoir and the method of Li-ion release.

Reviewer 3:

The reviewer noted that the program has ended.

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

Reviewer 1:

The reviewer said the project is highly relevant to the VTO battery program and directly addresses the problem of capacity fade with charge/discharge cycling due to Li consumption/depletion.

Reviewer 2:

The reviewer said that an in-operando solution for re-lithiation will reduce the cost associated with designing cells for long life, and exploratory study to understand the feasibility of such systems is important in understanding the risks and benefits of such approaches.

Reviewer 3:

The reviewer remarked the project can potentially address the issue of low Coulombic efficiency of some high energy electrode materials, and matches the DOE objectives.

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

Reviewer 1:

The reviewer said that funding is sufficient for completing the stated milestones.

Reviewer 2:

The reviewer remarked resources are sufficient.

Reviewer 3:

The reviewer said resources at the National Renewable Energy Laboratory (NREL) are sufficient to perform future project tasks.

Presentation Number: bat392
Presentation Title: Enabling Rapid Charging in Lithium-Ion Batteries via Integrated Acoustofluidics
Principal Investigator: James Friend (University of California at San Diego)

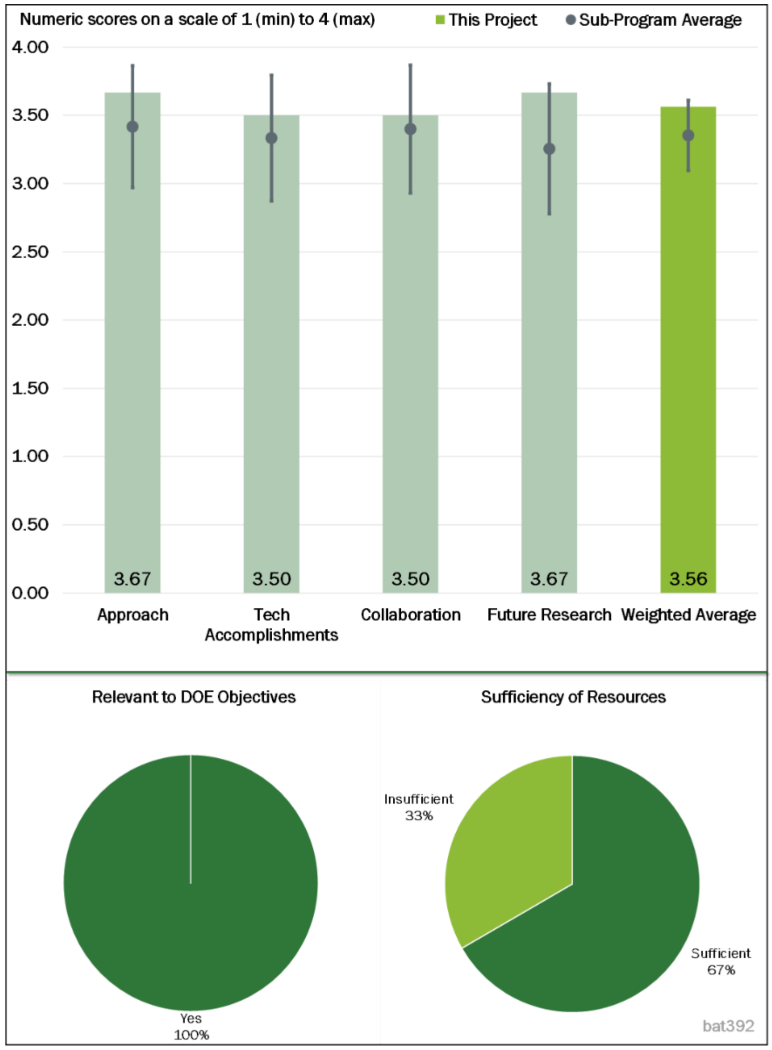

Figure 2-68 – Presentation Number: bat392 Presentation Title: Enabling Rapid Charging in Lithium-Ion Batteries via Integrated Acoustofluidics Principal Investigator: James Friend (University of California at San Diego)

Presenter

James Friend, University of California at San Diego

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 to the barrier is well designed and well executed, and that the approach requires close control of cell parameters during fast-charge, but this can be easily achieved with integrating the controls in the battery management system (BMS). The reviewer said it is a unique approach which show lots of promise for actual application.

Reviewer 2:

The reviewer remarked using acoustics to enhance Li-ion diffusion is a good idea, and the team has proved the concept.

Reviewer 3:

The reviewer said that the PIs use an intense surface acoustic wave during Li-ion battery charging to keep the electrolyte well mixed. The reviewer remarked the method is intended to overcome ion depletion during the anode surface during charging to prevent/minimize Li-metal plating, and the method is innovative and non-invasive. The reviewer said the PIs are directly addressing the problem of Li plating during fast charging 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 remarked significant progress has been made, and cell data show good improvement.

Reviewer 2:
The reviewer said the team has already integrated acoustic device into a pouch cell, and demonstrated enhanced capacity at fast charging.

Reviewer 3:
The reviewer commented that the PIs have shown good progress on the project. The reviewer noted that for a 2 A-h prototype pouch cell battery, the application of a surface acoustic wave (SAW) resulted in an improvement in the discharge capacity above 200 mA charge rates. Modulating the SAW (50% time on during charging) appears to work well. The reviewer noted that 100% SAW on results in a large drop in Coulombic efficiency, for reasons not well understood.

The reviewer detailed that a mathematical model of macro-transport near the anode surface with/without acoustic wave agitation was also developed. A Peclet number correlation was identified for predicting when the geometry (height) of surface asperities at the anode surface will result in Li-metal plating. The reviewer said the exact connection between the modeling work and experiments is not entirely clear, and asked how the model will be used to identify the best way to implement acoustic wave electrolyte agitation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said close collaboration with industry and other technical partners.

Reviewer 2:
The reviewer remarked the team is composed of a battery scientist, mechanical engineer, and circuit design company, and the team is collaborating effectively.

Reviewer 3:
The reviewer commented that collaborations are listed in the poster, but the exact contributions from the Technion and Stanford are 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 noted an excellent plan to increase the cell size to understand the effect of size. Improving the understanding of the mechanism by which the SAW device operates is important.

Reviewer 2:
The reviewer commented future research is well planned, although jelly roll configuration will be very different from pouch cell.

Reviewer 3:
The reviewer said that plans for future work are well conceived and reasonable. Future work will focus on transitioning from a prismatic pouch 2 Ah battery with SAW to a jellyroll configuration, with charging rates increasing from 3-4C to 6C. The reviewer noted an extension of the modeling work, and that more modeling work is also planned.

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

Reviewer 1:
The reviewer remarked rapid charging of a Li-ion battery, without Li-metal plating or irreversible capacity loss, is an important problem that needs to be addressed. Thus, this project is highly relevant to the DOE-EERE VTO program.

Reviewer 2:
The reviewer said the project can potentially address the issue of insufficient Li-ion diffusion at high charging rates, and matches the DOE objectives.

Reviewer 3:
The reviewer said it is relevant to extend the usability of cells over long life.

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

Reviewer 1:
The reviewer said that more resources will help to characterize the effect of this system over long-term operation, and to build it in large format cells.

Reviewer 2:
The reviewer said resources are sufficient.

Reviewer 3:
The reviewer remarked there are sufficient resources at the University of California-San Diego to achieve the project milestones in a timely fashion.

Presentation Number: bat393
Presentation Title: Development of an Extreme Fast Charging Battery
Principal Investigator: Chao Wang-Yang (Penn State University)

Presenter
Chao-Yang Wang, Penn State University

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

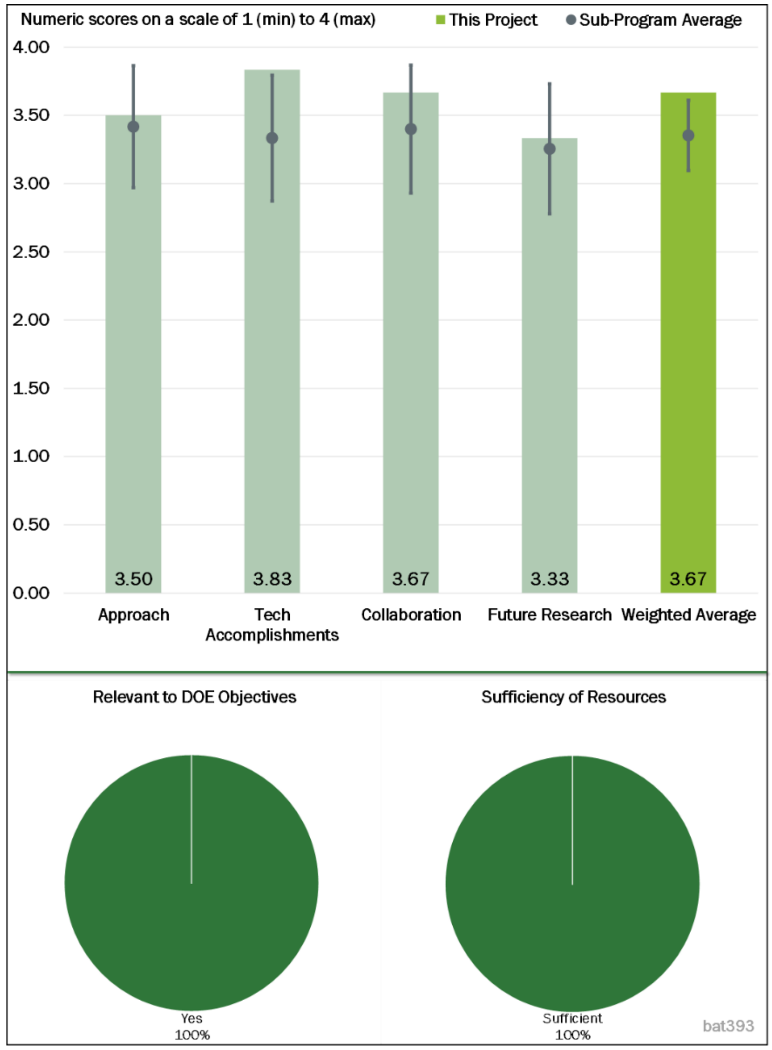

Figure 2-69 – Presentation Number: bat393 Presentation Title: Development of an Extreme Fast Charging Battery Principal Investigator: Chao Wang-Yang (Penn State University)

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 detailed that the PI is examining a new strategy for fast-charging a Li-ion cell at a high temperature (40-60°C) to eliminate Li plating. The cell stays at a high temperature only during charge (~10-min per cycle, corresponding to 6C). The team has developed a method for very rapid heating of the battery, at 1°C/sec. The reviewer found this to be a very simple and effective approach for fast-charging a Li-ion battery without Li-metal plating or a substantial capacity fade.

Reviewer 2:
The reviewer remarked the project is based on a very feasible idea, that can effectively enhance fast-charging performance.

Reviewer 3:
The reviewer said that the approach is unique and interesting. It does address the technical barriers for fast charging, but it requires significant change in cell design. The reviewer said it introduces challenges associated with high-temperature stability of cathodes.

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 made on this project during Year 1. The reviewer detailed that the PI developed a numerical model that can predict capacity loss induced by Li plating and SEI growth. The model shows that the onset of Li plating leads to rapid capacity fade, but charging at an elevated operating temperature postpones the onset of Li plating. The reviewer noted that a rapid heating device has been

incorporated into pouch cells. By elevating the charge temperature to 60ºC, the Gen-1 graphite/NMC extreme fast charging (XFC) cells (with an internal heater) retain 94% capacity after 1,800 cycles of 6C charge to 80% SOC. The reviewer said that in 35-Ah configuration, Gen-1 XFC cell gives a C/3 discharge energy of 170 Wh/kg after 6C charge to 80% SOC, which is close to the DOE target (180 Wh/kg).

Reviewer 2:
The reviewer remarked the team has made very good progress, that give the reviewer great confidence that this project will be a great success at the end.

Reviewer 3:
The reviewer said that technically, challenges have been sufficiently addressed. The design enables 6C fast-charge and long cycle life. The reviewer noted that calendar life stability needs to be explored.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said good partnership with collaborators.

Reviewer 2:
The reviewer commented that the team is composed of two Penn State faculty members, and an ANL scientist. Each team member has well-defined and justified contributions to the whole project.

Reviewer 3:
It appeared to the reviewer that there was no collaboration with Dr. Donghai Wang at Penn State and Dr. Zhengcheng Zhang at ANL during Year 1. Such collaborations may be important during Year 2.

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 work tasks are reasonable and are appropriate, given the excellent results in Year 1. The reviewer detailed that future tasks are first, fabricate extremely fast-charging cells with a higher anode loading (>4mAh/cm^2), where the cell-level energy density is greater than 225 Wh/kg; second, identify the optimal charging temperature to eliminate Li plating; and third, demonstrate that the Year 2 XFC cells will meet the DOE target of a C/3 discharge energy greater than 180 Wh/kg after 10-mininue fast-charge. The reviewer pointed out that it may be necessary to develop new electrolytes and additives that can improve the thermal stability of the anode, if the charging temperature is to be further increased above 60ºC.

Reviewer 2:
The reviewer noted that NMC811 stability for high-temperature is most concerning. The reviewer said that temperature distribution in a large format cell needs to be addressed.

Reviewer 3:
The reviewer suggested the team add cost analysis into future work.

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

Reviewer 1:
The reviewer remarked that fast-charging of a Li-ion battery, without Li-metal plating or irreversible capacity loss, is an important problem for battery developers that needs to be addressed. It is critical for expanded electrical vehicle use. Thus, per the reviewer, this project is highly relevant to the DOE-EERE VTO program.

Reviewer 2:
The reviewer said that the project is relevant to explore the effects of such integrated solutions at the cell level.

Reviewer 3:
The reviewer said that the project uses a simple device to enable a self-heating function to battery to address the kinetics issue, and matches the DOE objective of fast charging.

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 funding levels are sufficient.

Reviewer 2:
The reviewer remarked the resources are sufficient.

Reviewer 3:
The reviewer commented there are sufficient resources at Penn State University to achieve the project milestones.

Presentation Number: bat394
Presentation Title: Highly Ordered Hierarchical Anodes for Extreme Fast-Charging Batteries
Principal Investigator: Neil Dasgupta (University of Michigan)

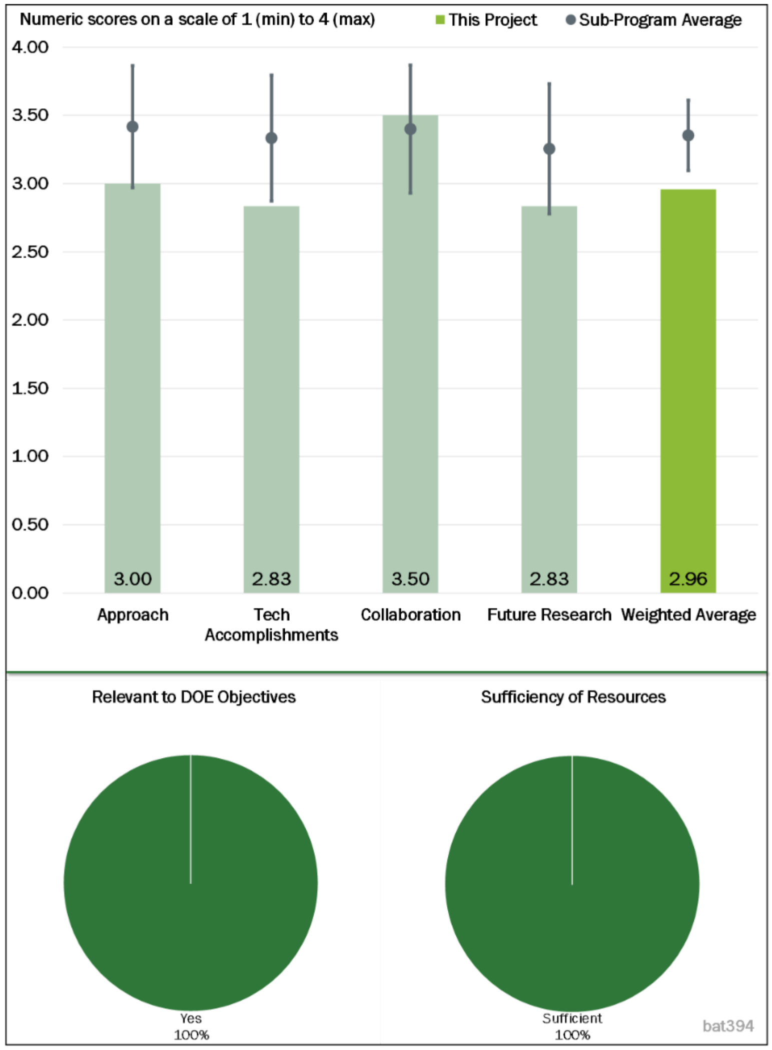

Figure 2-70 – Presentation Number: bat394 Presentation Title: Highly Ordered Hierarchical Anodes for Extreme Fast-Charging Batteries Principal Investigator: Neil Dasgupta (University of Michigan)

Presenter

Neil Dasgupta, University of Michigan

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 approach addresses Li mobility in thick electrodes for fast-charge.

Reviewer 2:

The reviewer said the PI uses a laser patterning method to create highly ordered hierarchical (HOH) architecture anodes where open channels are formed through the anode layer in the thickness direction. Such channels allow for better electrolyte infiltration into the anode for fast-charging. The reviewer said the project involves multiple PIs, with anode development and manufacturing, computational modeling, and electrode characterization tasks.

Reviewer 3:

The reviewer remarked price and time increases due to the added laser processing should be quantified.

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 fast-charge goals of 80% SOC in 10 minutes are not met. Long-term cycling effects of fast-charging needs to be addressed.

Reviewer 2:

The reviewer said drilling holes have improved the performance, but is still away from the target numbers (180 Wh/kg at 3C, 500 cycles with less than 20 capacity fading). With holes, electrodes have to be made thicker to have the same areal capacity.

Reviewer 3:

The reviewer described that a laser ablation process has been developed for rapid and scalable modification of pouch-cell-sized electrodes. Anodes were modified by the laser ablation method, where the hole spacing and diameter was varied and the resulting anodes were characterized. The reviewer remarked that the effect of anode architecture on the rate capability and Li plating in graphite and hard carbon anodes was evaluated. The improvement in capacity for fast-charging rates was modest. Graphite anodes (3 mAh/cm^2 areal loading) with a 10-minute charge (6C) showed a capacity retention of only 55% for the patterned anode versus. 43% for a conventional anode. Also, noted the reviewer, some of the Year 1 milestones were not discussed, e.g., ALD LTO coatings of patterned anodes. The reviewer asked if such experiments were performed.

The reviewer does not see how the PIs will meet their goal of a 10-minute fast charge protocol at 500 cycles with less than 20% fade in capacity. Current results fall far short of this goal and the reviewer does not see how the perforated anode architecture will dramatically improve the capacity retention during fast charge. Having a perforated anode does not induce any kind of electrolyte flow; the reviewer asked so how will further changes to anode geometry create very large changes in capacity at fast-charging rates.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said good partnership with collaborators.

Reviewer 2:

The reviewer remarked the team has demonstrated active collaboration, from fabrication, modeling, to diagnosis.

Reviewer 3:

The reviewer noted that wide-ranging collaborations are listed in the slides, with Sandia National Laboratories (SNL), ANL, NREL, Stanford Linear Accelerator Center (SLAC), and ETH Zürich. The reviewer said it is not clear which collaborators contributed to the project during Year 1.

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 research is well planned.

Reviewer 2:

The reviewer said that greater than 180Wh/kg should be the key target to achieve over long-term cycling with fast-charge protocol.

Reviewer 3:

The reviewer detailed that future experiments will focus on first, manufacturing greater than 2Ah prototype batteries with the patterned electrode architecture which exhibit a 200% improvement in capacity retention at 4C and 100% improvement of capacity retention at 6C over 100 cycles (this will be a challenge, given the modest capacity improvement seen to date); second, demonstrating improved interfacial kinetics and homogeneity of Li insertion across the electrode/electrolyte interface using atomic layer disposition (ALD) treatments (the reviewer does not see how this task will help in achieving Task No. 1); and third, developing an improved fundamental understanding of Li plating on graphite using operando video microscopy and Raman spectroscopy (again, the reviewer does not see how these experiments will improve/help in improving the design/operation of patterned electrodes during fast-charging).

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

Reviewer 1:
The reviewer pointed out that fast-charging of Li-ion batteries is an important and timely problem to address. The subject matter of this project is highly relevant to the DOE-EERE VTO program.

Reviewer 2:
The reviewer said that understanding the effect of three-dimensional (3D) architecture electrodes is important for fast charge and high energy cells.

Reviewer 3:
The reviewer remarked the project can potentially address the ion diffusion to the bottom of thick electrodes, and matches the DOE objectives.

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

Reviewer 1:
The reviewer said that resources are sufficient.

Reviewer 2:
The reviewer remarked the team has sufficient resources.

Reviewer 3:
The reviewer said that there are sufficient resources to achieve the project milestones.

Presentation Number: bat395
Presentation Title: Developing Safe, High-Energy, Fast-Charge Batteries for Automobiles
Principal Investigator: Bryan Yonemoto (Microvast, Inc.)

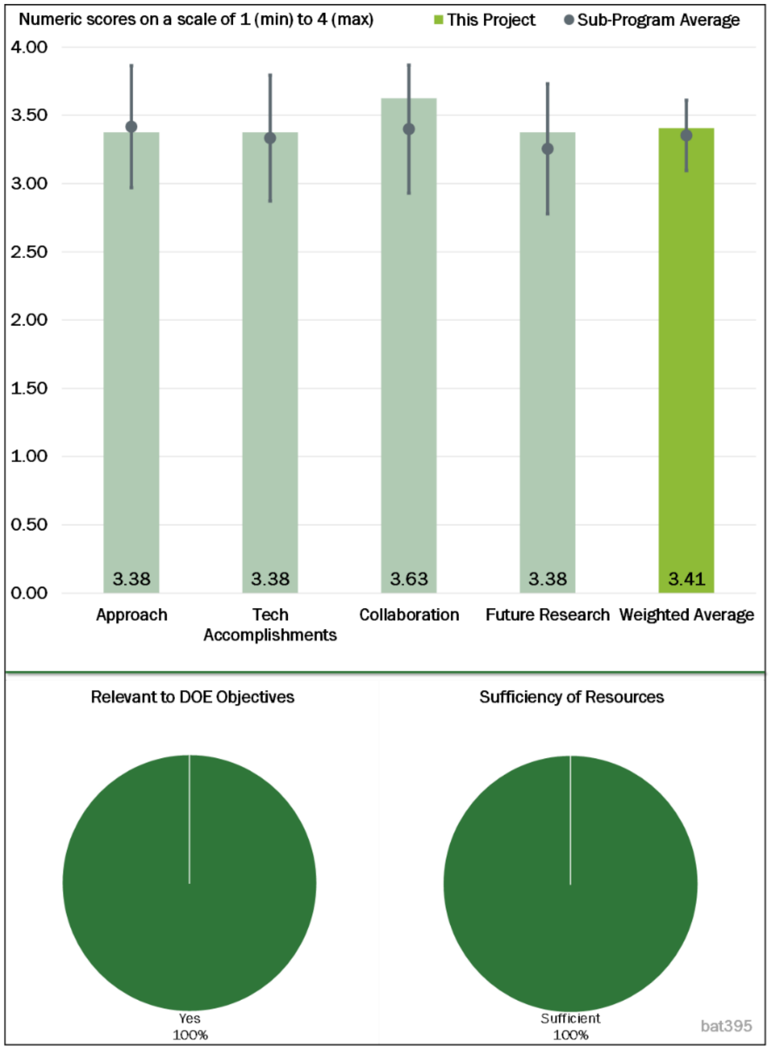

Figure 2-71 – Presentation Number: bat395 Presentation Title: Developing Safe, High-Energy, Fast-Charge Batteries for Automobiles Principal Investigator: Bryan Yonemoto (Microvast, Inc.)

Presenter
Bryan Yonemoto, Microvast, Inc.

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 approach was well designed.

Reviewer 2:
The reviewer remarked the approach is novel and well positioned to address the barriers for XFC, and high-energy and safe batteries. The team consists of Microvast, Inc. (lead), ANL, and BMW, with complementary expertise.

Reviewer 3:
The reviewer detailed that new cathode and electrolyte materials will be used in Generation-1 and Generation-2 Li-ion pouch and prismatic large format automotive cells for fast-charging. The project looks at cathode catalyst development to increase the energy density of Li-ion batteries. The reviewer remarked it appears that the emphasis of this project is on materials development for high-capacity cells, although fast-charging will be tested and studied.

Reviewer 4:
It is not clear to the reviewer that the reported approaches will enable fast-charging. There lacks a rationale of the design.

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 program met all the project goals.

Reviewer 2:
The reviewer remarked this is the first year and the team has accomplished much in terms of milestones. The project is on track and in good shape.

Reviewer 3:
The reviewer said that to date, project milestones have been met. The reviewer noted that 15 AH cells have met the project's performance target, with more than 90% capacity retention after 500 cycles of 10-minute fast charge, 1C discharge (the project goal is a capacity loss less than 20% after 500 cycles). The listed 2018 Go/no-go decision point on Slide 3 is the delivery of 20 AH cells (Gen-1, ~220 Wh/kg) that pass 500 XFC cycles. The reviewer pointed out that this was not yet accomplished. On Slide 4, this same target is listed as a 2019 go/no-go. So, it is not clear as to the timing of this important metric. The reviewer said that as of the AMR, the capacity retention of 22 AH (220 Wh/kg) cells was near, but below the 80% target. The project successfully assembled hard can cells (180 Wh/kg) using Microvast FCG cathode and graphite anode in PHEV1 format (24 Ah). Also, Generation-1 and Generation-2 cathode materials were developed and characterized. The reviewer said that progress has been good, and the PI needs to better explain if the go/no-go was met. There was no discussion/analysis of possible Li plating on the cathode. The reviewer asked if this is an issue that need to be addressed.

Reviewer 4:
The reviewer commented that so far, all the reported data of this project are using low rate, not fast charging. The reviewer is not sure if the concepts will work at a high rate (e.g., 3C).

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer said good collaboration with industry partners.

Reviewer 2:
The reviewer commented that this is an excellent team work with industry and a National Laboratory. The team has been collaborating to deliver the milestones and use the resources in each site.

Reviewer 3:
The reviewer remarked the team has demonstrated active collaboration.

Reviewer 4:
The reviewer said there is demonstrated evidence of very good collaboration with ANL (development and characterization of cathode materials) and BMW (building hard can jelly roll cells and developing advanced fast-charge protocols).

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

Reviewer 1:
The reviewer pointed out that the plan is to achieve energy density in large format cells.

Reviewer 2:
The reviewer remarked the future plan is solid. The team has characterized the cathode and obtained a fundamental understanding of the mechanisms which help improve the cells in Year 2.

Reviewer 3:
The reviewer noted that the PI lists the Generation-1 fast-charging cell go/no-go decision test as a future work task. The reviewer asked if this will be the 20 AH (220 Wh/kg) cell. Future work includes the delivery of fast-charging cells to a National Laboratory for testing. Both Generation-2 and Generation-3 cells will be built and tested, but it is not clear what the anticipated improvements will be in these new cells. The reviewer wondered if the anticipated improvements would be better capacity retention after 500 cycles, higher initial capacity, the use of a different fast charging protocol, etc.

Reviewer 4:
The reviewer commented the team has not made it clear in the future work section how it would achieve fast charging.

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

Reviewer 1:
The reviewer pointed out that fast-charging of high-capacity Li-ion batteries is an important problem that needs to be addressed. Thus, this project is highly relevant to the DOE-EERE VTO program.

Reviewer 2:
The reviewer said that cathode development to achieve fast charge is very relevant.

Reviewer 3:
The reviewer noted that this project addresses the urgent need for XFC batteries. The project has the potential to achieve the DOE targets and transfer the technologies to industry to enable at-scale production.

Reviewer 4:
The reviewer commented that if successful, this project can potentially increase the energy density (not sure about fast charging) of Li ion batteries, and matches the DOE objectives.

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

Reviewer 1:
The reviewer said that funding is sufficient.

Reviewer 2:
The reviewer remarked the team has efficiently used the resources at each site and leveraged the facilities and expertise.

Reviewer 3:
The reviewer commented the team has sufficient resources.

Reviewer 4:
The reviewer found that there are sufficient resources to achieve the project milestones in a timely fashion.

Presentation Number: bat396
Presentation Title: Enabling Extreme Fast Charging through Anode Modification
Principal Investigator: Esther Takeuchi (Stony Brook University)

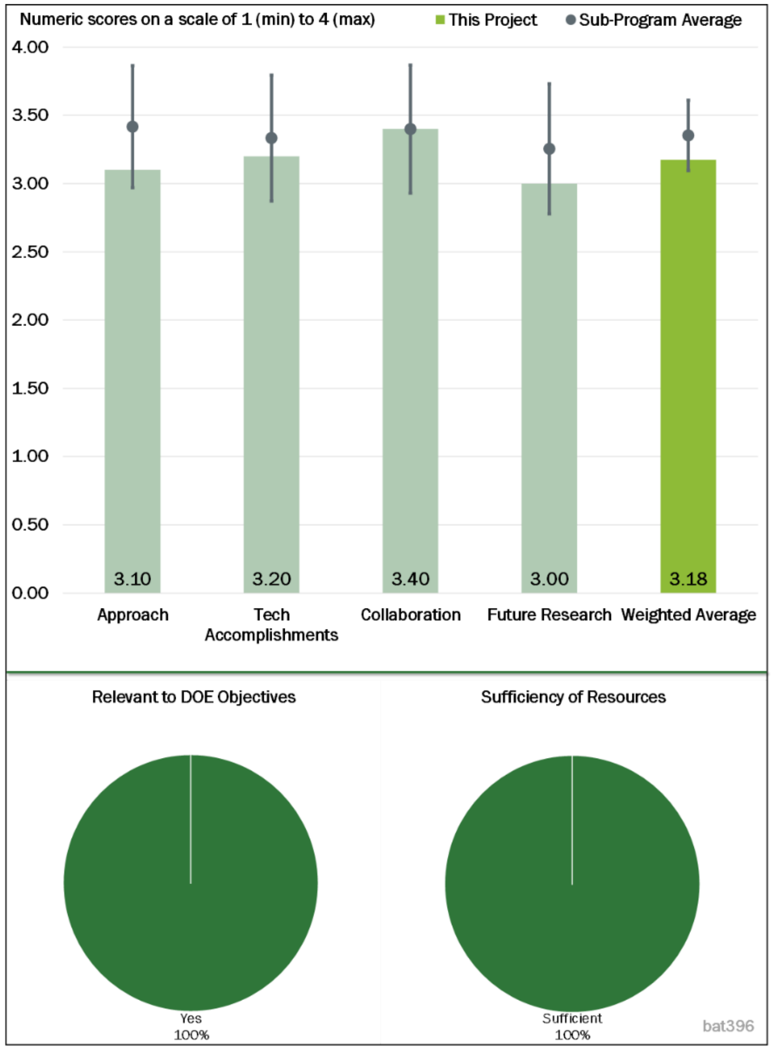

Figure 2-72 – Presentation Number: bat396 Presentation Title: Enabling Extreme Fast Charging through Anode Modification Principal Investigator: Esther Takeuchi (Stony Brook University)

Presenter

Esther Takeuchi, Stony Brook 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 remarked that the objective here is to develop a surface treatment for the graphite anode that will provide high overpotential for Li deposition and enable XFC without the problem of Li plating. The expectation is that a modification of graphite substrate with a thin (nanometer) coating of suitable coating will hinder Li plating without impacting Li intercalation kinetics within graphite anode. The reviewer said that this approach is novel and based on good electrochemical reasoning. Using graphite anodes with selected surface coatings, Li-ion pouch cells were made with NMC cathodes and tested to show that the surface coatings have not altered the graphite performance characteristics. The reviewer noted that fast recharge capability is not yet demonstrated, but Li plating behavior was evaluated by constant voltage charging at low anode potentials (below Li potentials) and the plated Li was estimated relatively from the X-ray diffraction spectroscopy (XRD) of standard and coated graphite anodes. The reviewer said the project is well designed to address the fast-charging issue of Li-ion cells and is consistent with the goals of DOE's VTO. The project is well integrated with the other VTO projects also and may easily be implemented together with other cell modifications.

Reviewer 2:

The reviewer remarked that because the metal coating is done after forming the electrode, and it will not prevent electrolyte from penetrating into the electrode, the reviewer is not sure if Li-metal will still plate inside the thick electrode.

Reviewer 3:

The reviewer said that the approach to date has demonstrated measurable results in line with project milestones and schedule. Next step barriers are identified with a reasonable path ahead.

Reviewer 4:
The reviewer said that metallic Li plating during fast charging was addressed effectively through Li deposition overpotential control with nanometer scale surface coating on graphite. The reviewer said that the approach seems adequate to address the Li plating issue. However, it is unclear to this reviewer if the coating will affect battery discharge power at high rate.

Reviewer 5:
The reviewer remarked uniform surface coating on electrode material is a complicated process. Graphite-metal interface needs to be studied to understand the reactions that form SEI, and inhibition to plate Li at high rate should be explored first.

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 the progress toward individual milestones and the upcoming go/no-go decision has established measurable properties of baseline and surface enhanced trial cells. The reviewer said repeatable C/2 charging and the respective results toward the 50-cycle target is an open question, but results to date are encouraging.

Reviewer 2:
The reviewer remarked reasonably good progress has been made overall. Using commercially available materials, two different surface coatings of ~10 nm have been examined on the graphite anode. The uniformity of the surface coating has been verified using different analytical techniques and the performance containing treated and untreated graphite electrodes has been demonstrated in half-cells. The reviewer said that the surface coatings did not show any impact on the capacity or Coulombic efficiency, nor increased the impedance. However, the cycle life is rather poor with more than 20% capacity loss in 100 cycles (in all the cases). Initial Li plating behavior was evaluated by potentiostatic charging at a lower potential experiment (the reviewer asked why not the conventional galvanotactic charging at a current density corresponding to 4-6C charge rate?) and the coated graphite anodes showed reduced Li plating on surface treated graphite compared to untreated graphite. The reviewer remarked it would be useful to evaluate this at different SOCs of the graphite anode and to identify more quantitative method for determining the plated Li. Further, some information on the anticipated overpotentials for Li deposition would be useful, since this was the guiding principle for this proposal. The reviewer was unsure if the full cells were made in June as shown in the schedule (around the AMR). Overall, the progress achieved here is meaningful and relevant to DOE's goals.

Reviewer 3:
The reviewer said that reasonable progress has been achieved within a limited time and it has been proved that surface treated electrodes have reduced Li plating relative to uncoated graphite. However, so far there is no significant difference for battery capacity retention of untreated and treated graphite at C/2 rate. The reviewer was unclear if the higher charging rate will show the difference for coated and uncoated anodes.

Reviewer 4:
The reviewer remarked the chemical and electrochemical characterization of the prepared material show very small variation from baseline.

Reviewer 5:
The reviewer remarked that fast-charging (e.g., 3C) is still yet to be demonstrated.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer commented the team has demonstrated active collaboration.

Reviewer 2:

The reviewer remarked there is good on-going collaboration with Brookhaven National Laboratory (BNL) (National Synchrotron Light Source II, Center for Functional Nanomaterials) for metal film deposition and characterization and BNL for cell characterization efforts.

Reviewer 3:

The reviewer observed good collaboration with National Laboratories.

Reviewer 4:

The reviewer remarked the team formed with a university and a National Laboratory is well designed for the efforts

Reviewer 5:

The reviewer said collaboration between team members looks effective and the demonstrated results between the groups toward objective to date seem effectively orchestrated.

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 planned future work aligns well with the established objectives and milestones with the near-term go/no-go decision point providing a pivotal technical metric for the project.

Reviewer 2:

The reviewer said that the proposed future research addresses current challenges and batteries to minimize Li plating. Battery capacity retention at high rate may also need to be addressed to demonstrate positive impact of the battery with coated graphite on battery life under fast-charging condition.

Reviewer 3:

The reviewer pointed out that being a new project, a few challenges still remain, i.e., to optimize the surface coating (material selection, thickness) for mitigating Li plating during fast charge. The future studies of preparing and characterizing surface treated graphite electrodes at three different thicknesses and performing Li plating experiments with quantification of deposited Li by XRD, building test Li-ion cells with and without coated anodes to evaluate fast charging capability versus control cells are logical. The reviewer pointed out that the best aspect of this technology (surface coating on graphite) is that it can be easily implemented in full cells in conjunction with other cell developments in the VTO program. To that end, it is important to identify a manufacture-friendly (for scale up) method for the surface treatment of graphite.

Reviewer 4:

The reviewer remarked that electrolyte development to optimize SEI formation should be a key point of future work.

Reviewer 5:

The reviewer suggested battery cycling at a higher rate, because fast charging is the main focus of this program. Also, the reviewer suggested the team report more performance metrics, such as overall specific energy of the cells. The reviewer also suggested pouch cells be tested and reported.

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

Reviewer 1:
The reviewer said that for a widespread use of EVs, batteries with higher energy and lower cost than the current Li-ion batteries and reduced charging time (15 minutes or less) are needed. New approaches to mitigate Li plating during fast charge are desired to meet the goals of DOE, which this project has been addressing.

Reviewer 2:
The reviewer remarked it is relevant to explore new options to prevent Li plating.

Reviewer 3:
The reviewer said this project is very helpful for DOE's goal to increase battery charging time while reducing Li plating.

Reviewer 4:
The reviewer commented the project can potentially address the issue of fast charging, and matches DOE objectives.

Reviewer 5:
The reviewer said this project's foundation is rooted in the DOE's target of XFC battery cells. While the capability to demonstrate this is planned within the program, the limit of delivering such results only at a 2Ah cell deliverable is limiting (but realistic for non-industry development).

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

Reviewer 1:
The reviewer commented the personnel and collaborative facilities to accomplish the goals of this project seem realistic to meet the target end-program deliverables.

Reviewer 2:
The reviewer said that resources are appropriate for the scope of the project

Reviewer 3:
The reviewer found that funding is sufficient for this work.

Reviewer 4:
The reviewer said that resources seem sufficient to conduct the remaining work.

Reviewer 5:
The reviewer remarked the team has sufficient resources.

Presentation Number: bat397
Presentation Title: Titanium Niobium Oxide-Based Lithium-Ion Batteries for Extreme Fast-Charging Applications
Principal Investigator: Sheng Dai (University of Tennessee at Knoxville)

Presenter

Sheng Dai, University of Tennessee at Knoxville

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 remarked that the approach leveraging titanium niobium oxide (TNO) fabrication techniques addresses electronic conductivity enhancement and potentially provides a path toward achieving project objectives of capacity improvements for XFC applications.

Reviewer 2:

The reviewer said that using TNO as an anode does avoid the Li-metal plating, but will significantly reduce the average full cell voltage, down to 2.1 volt (V) due to the high working potential of TNO. The reviewer suggested the team report the specific energy of their full cells.

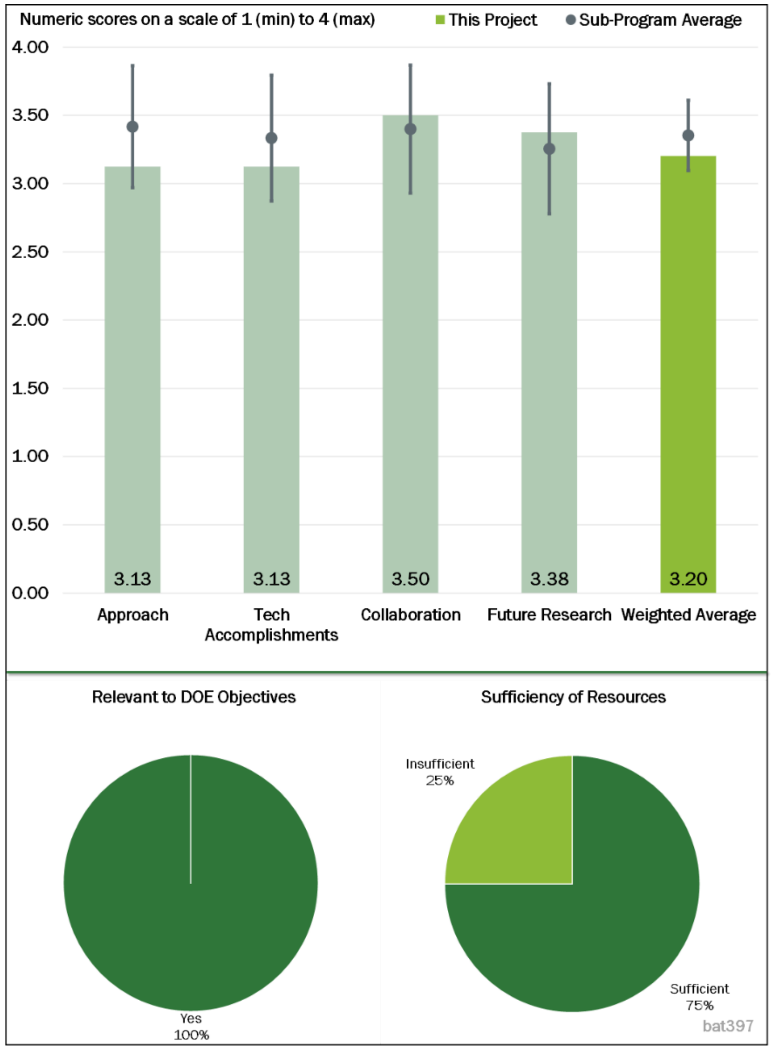

Figure 2-73 – Presentation Number: bat397 Presentation Title: Titanium Niobium Oxide-Based Lithium-Ion Batteries for Extreme Fast-Charging Applications Principal Investigator: Sheng Dai (University of Tennessee at Knoxville)

Reviewer 3:

The reviewer remarked the effort of developing a TNO-based anode may well address the battery charging and capacity retention issues. However, the limited specific energy density due to narrow working voltage range for the battery with TNO may limit its application.

Reviewer 4:

The reviewer said that achieving target energy density is a challenge 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 pointed out the team achieved a 10-minute charge for over 250 cycles.

Reviewer 2:
The reviewer said the team has achieved interesting progress and fast charging was demonstrated to be feasible for TNO anode-based coin cells.

Reviewer 3:
The reviewer remarked the progress to date establishes the viability of synthesizing porous TNO and carbon-coated TNO, although the details on the process could be further established. Additionally, the demonstration of high charge rate shows the value in the team's approach, although to date the 4C rate is the optimal result.

Reviewer 4:
The reviewer found that the progress on material synthesis and characterization has been satisfactory. However, specific energy of the full cell, as well as areal capacity, needs to be reported. The reviewer said these two numbers seem to be low in the current report.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer observed outstanding collaboration with the project team.

Reviewer 2:
The reviewer remarked the team consisting of university, National Laboratory, and industry partners is well designed to conduct the research work.

Reviewer 3:
The reviewer said the team has demonstrated active collaboration.

Reviewer 4:
The reviewer said it is demonstrated that cell fabrication and characterization between the University of Tennessee (UT) and ORNL has produced positive progress in the program. The effort to establish collaborative depth with the active material suppliers seems adequate to acquire the necessary components, but discussion on optimizing said materials for the fabrication approach is limited.

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 the future work is inclusive of total development to achieve high-energy, fast cell and large format cells.

Reviewer 2:
The reviewer said the proposed future work is adequate and NMC/TNO-based pouch cells will be made and tested.

Reviewer 3:
The reviewer commented the proposed future work provides a path toward evaluating the project's technical approach to meet each milestone and objective, although the timeline seems aggressive for the remaining work.

Reviewer 4:
The reviewer said that future work is missing metrics on specific energy of the full cell.

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

Reviewer 1:
The reviewer said that the project supports overall DOE objectives.

Reviewer 2:
The reviewer remarked battery fast-charging is addressed by this project, and a TNO-based coin cell was made and tested.

Reviewer 3:
The reviewer said, if successful, the project can potentially address the issue of Li plating at fast charging, and matches the DOE objectives.

Reviewer 4:
The reviewer remarked the project addresses the DOE's challenge of leveraging a chemistry to meeting XFC capabilities, although the targeted deliverables may only provide an initial insight toward full cycle life and abuse tolerance.

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 more funding would be needed to develop large format cells.

Reviewer 2:
The reviewer said there was no indication that new resources are needed for this project.

Reviewer 3:
The reviewer said the team has sufficient resources.

Reviewer 4:
The reviewer remarked the project's access to the necessary materials, knowledge to fabricate the targeted electrode structures, and characterize the scaled prototype cells seems sufficient.

Presentation Number: bat398
Presentation Title: Extreme Fast-Charging Lithium-Ion Batteries
Principal Investigator: Edward Buiel (Edward Buiel Consulting, LLC)

Presenter

Edward Buiel, Edward Buiel Consulting, LLC

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.

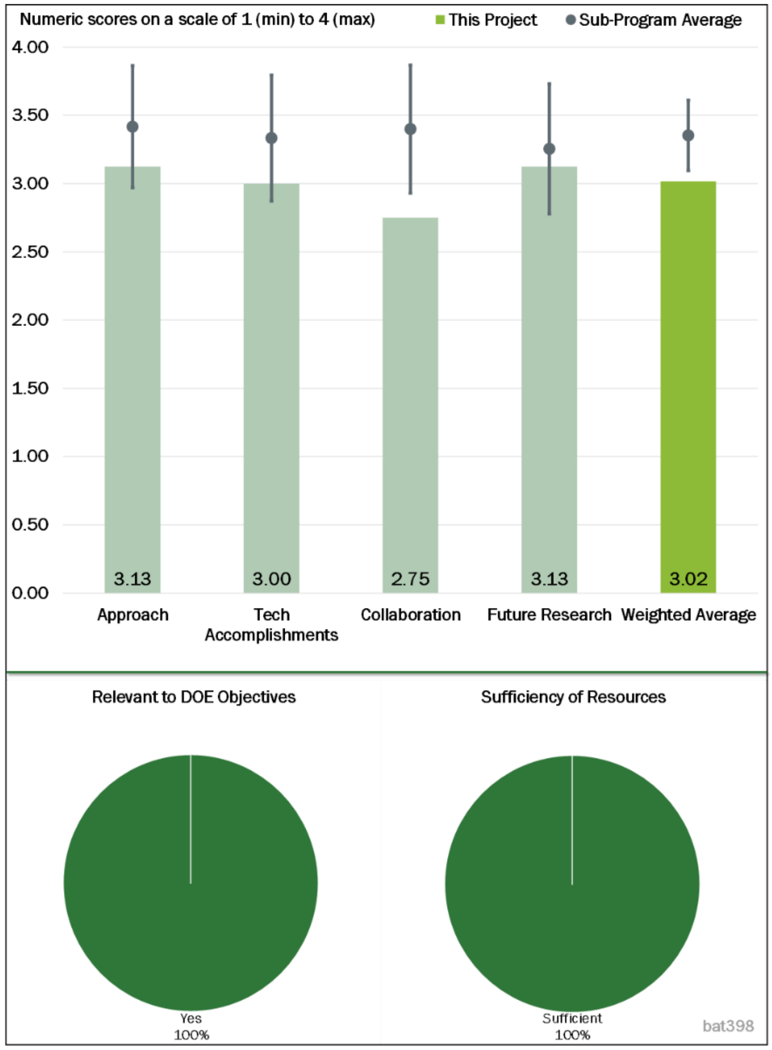

Figure 2-74 – Presentation Number: bat398 Presentation Title: Extreme Fast-Charging Lithium-Ion Batteries Principal Investigator: Edward Buiel (Edward Buiel Consulting, LLC)

Reviewer 1:

The reviewer remarked it is a good approach to design new anode material, conducting cell optimization, and perform electrolyte optimization for battery XFC.

Reviewer 2:

The reviewer remarked the project has a novel approach with the goal to develop XFC Li-ion batteries. The results from budget period 1 are solid and promising. The reviewer noted that the first year has accomplished much in terms of anode material development, cell design optimization, and electrolyte optimization.

Reviewer 3:

The reviewer said the approach gives a high-level path toward small format cells that may achieve the target energy density and demonstrate, at least, beginning of life (BOL) XFC charge rates. The reviewer pointed out that the approach on cell design and electrolyte optimization provides sparse details.

Reviewer 4:

The reviewer said that the objective here is develop anode materials to comply with the fast-charge capability of 6C over the entire life of the EV battery, without impacting the specific energy (greater than 144 Wh/kg). The strategy is to develop the anode material development, optimize the electrolyte and cell design, and build 18650 test cells with these modifications and test them under the DOE’s fast charge protocol and establish the Li plating onset behavior. The reviewer remarked Li-ion power cells with four different anode materials have been built and tested for first cycle Coulombic efficiency and area-specific impedance. No details are provided on the electrode parameters or the electrolytes incorporated in these cells. The reviewer noted that the go/no-go milestone (due in August 2019 but claimed to have been completed months in advance) calls for a lower specific energy of 120 Wh/kg, below the project goal of 144 Wh/kg. The reviewer said that it is rather difficult to assess the validity of approach without much of these details.

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 preliminary results showed cell impedance reduction through cell optimization and anode material formulation. There are no data presented to demonstrate reduced Li plating.

Reviewer 2:

The reviewer found that the project has accomplished the milestones of budget period 1. The project is on track and in good shape, and the anode development is promising.

Reviewer 3:

The reviewer remarked that progress to date, as presented, highlights improvements and approximate technical demonstration of budget period 1 energy density targets as well as high charge rate capability. The amount of XFC charge cycles is not provided, thus current claims of "long life" cannot be substantiated.

Reviewer 4:

The reviewer said that reasonably good progress has been made so far in this project. Representative 18650 Li-ion cells that can support fast charge rates were produced. The impedance of these cells was reduced by 42% through optimized cell design techniques and by 22% through optimized anode material and formulation. The reviewer remarked that even with the reduction in impedance, it is not clear if these cells can meet the fast-charge requirements of 6C. It is surprising as to why these cells have been subjected to these tests yet, at least to get baseline data. The reviewer was unclear what the specific energy is for these cells (~120 Wh/kg?) and how it will be improved to 180 Wh/kg in Build 2. It is difficult to assess the progress achieved without much of these details.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that there are no on-going collaborations yet, but Coulometrics is planning to manufacture XFC batteries in Chattanooga, Tennessee, using the technology developed here, and hopes to provide the batteries to automotive original equipment manufacturers (OEMs), power tool companies, and defense contractors

Reviewer 2:

The reviewer said that the project did not show collaboration. The reviewer suggested that the project perform atomistic and microstructural simulations to gain an in-depth understanding of XFC, which should in turn help the cell design and electrode selection.

Reviewer 3:

The reviewer remarked collaboration claims are unclear in the level of coordination beyond efforts within Coulometrics to produce cells internally with potential customers in medical devices, automotive OEMs, power tools, and defense. These entities seem to only provide potential application specifications.

Reviewer 4:

The reviewer pointed out that the project claimed there is a company that is going to license the developed technology. This is a single member team and they do not have an official partner.

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 plan of completing full cell homologation of optimized and cell is adequate.

Reviewer 2:

The reviewer remarked that the proposed future work makes sense. The project may explore atomistic modeling to understand the mechanisms.

Reviewer 3:

The reviewer remarked the proposed future studies of completing the material and cell optimization work are consistent with project goals. Subsequent to the material and cell optimization, full cell homologation will be implemented in subsequent cell builds, which expectedly produce batteries that exhibit long life and limited resistance increase over the life of the cell.

Reviewer 4:

The reviewer said that future work focuses on various high-level optimization approaches with encouraging potential to achieve the target energy density, but the reviewer is unclear how these efforts will ensure high XFC cycle life.

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

Reviewer 1:

The reviewer pointed out that for a widespread use of EVs, batteries with higher energy and lower cost than the current Li-ion batteries and reduced charging time (15 minutes or less) are needed. New materials and cell designs are required to mitigate Li plating during fast charge and meet the goals of DOE, which this project has been addressing.

Reviewer 2:

The reviewer commented the project addresses the urgent need for XFC and supports the overall DOE objectives. The budget period 2 should help at-scale production.

Reviewer 3:

The reviewer said that this project addresses the new graphite design that facilitates fast charging, which meet DOE's goals

Reviewer 4:

The reviewer remarked this project provides technical insight into cell development efforts toward achieving 6C-capable XFC 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 resources are okay for the efforts of this project.

Reviewer 2:

The reviewer commented the project has used the resources available at the company, which is sufficient for the project.

Reviewer 3:

The reviewer said that resources are bordering between sufficient and excessive, Coulometrics' growing manufacturing capability provides a unique capability to many other programs.

Reviewer 4:

The reviewer pointed out that budget information is not provided in this presentation.

Presentation Number: bat399
Presentation Title: High-Quality Natural and Synthetic Graphite for Lithium-Ion Batteries
Principal Investigator: Edward Buiel (Edward Buiel Consulting, LLC)

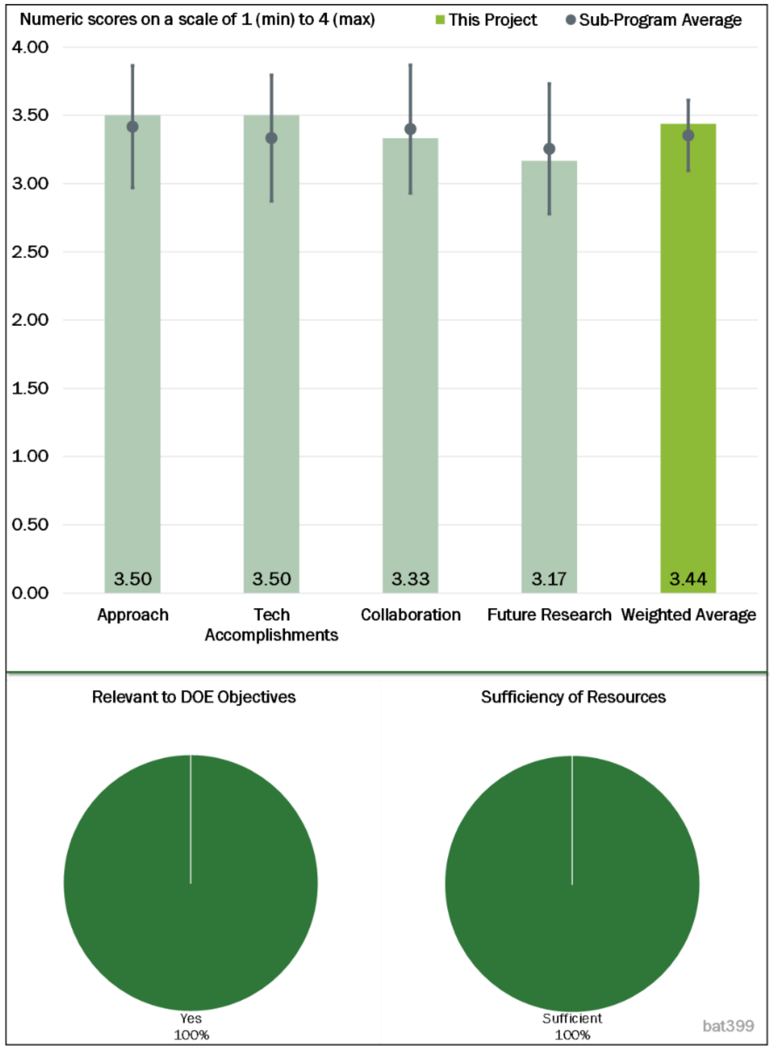

Figure 2-75 – Presentation Number: bat399 Presentation Title: High-Quality Natural and Synthetic Graphite for Lithium-Ion Batteries Principal Investigator: Edward Buiel (Edward Buiel Consulting, LLC)

Presenter
Edward Buiel, Edward Buiel Consulting, LLC

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 found that the approach is novel and covers a lot, and the systematic study of natural and synthetic graphite is of great importance for low-cost high performance Li-ion batteries.

Reviewer 2:
The reviewer remarked the combination of objectives, details, and general approach review establishes a focused technical scope to address the noted challenges.

Reviewer 3:
The reviewer said that the objective here is to develop a low-cost graphite for Li-ion batteries. The approach is to determine the effects of graphite particle morphology, density, and size on battery life, and charge rate capability, to minimize co-intercalation of electrolyte; to develop a surface coating in lieu of electrolyte additives; to develop slurry formulation for producing dense graphite anodes; and to fabricate and test 18650 (or 1 Ah pouch) cells for material validation. The reviewer was not clear if a CVD-coating of graphite is a preferred process to the addition of electrolyte additive, which is easier to implement and more robust in terms of surface coverage. The reviewer remarked the project is well-designed, and the approach looks feasible and well-integrated with other Vehicle Technologies Office (VTO) efforts. The reviewer noted that the only critical item that is missing here (in the presentation) is the cost analysis (must have been done) to show that the graphite produced here is indeed 50% cheaper than from commercial sources.

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 accomplished much in terms of milestones, and the systematic study on graphite should help optimize the cell configuration and performance. The project is in good shape to achieve the cost reduction of less than $5/kg.

Reviewer 2:

The reviewer commented with little remaining in the project, the accomplishments to date exhibit competitive performance with generalized cost benefits ("50% cost reduction over conventional graphite production processes used in Asia today" versus "<$5/kg" technical barrier).

Reviewer 3:

The reviewer found that good progress has been made overall. Impressive performance was shown by the graphite electrodes with high reversible capacity and low irreversible capacity, and more impressively, the 18650 cells performing as well during cycling at 40ºC (in comparison to Tesla batteries). The reviewer remarked that one curious thing to know would be the specific energy of these 18650 cells. It is also claimed that the Coulometrics' process would cost 50% lower than conventional graphite production processes currently used in Asia today. The reviewer remarked that overall, the progress achieved here is meaningful, significant, and relevant to DOE goals.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the project has a collaboration with PUREGraphite, which helps accelerate the progress.

Reviewer 2:

The reviewer remarked that the creation of the PUREgraphite joint venture seems to be an efficient method toward bringing the results to commercialization. DOE VTO and Coulometrics should further discuss the tech-to-market approach/opportunities.

Reviewer 3:

The reviewer noted that there is a good partnership between Coulometrics and PUREgraphite, which is their joint venture to commercialize and produce high-performance anode materials. PUREgraphite has plans to install production capabilities for 1,000 tons per year of graphite anode material that will be operational by fourth quarter 2019. The reviewer pointed out that collaborations with the National Laboratories or other sources for performance validation of the graphite anodes and Li-ion cells would be 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 said that the proposed future research is well positioned to achieve the objectives. The project may explore atomistic simulations to understand the mechanisms of graphite in high-performance batteries.

Reviewer 2:

The reviewer said that despite the successful results that far, it is essential to address the critical challenges related to the development of an environmentally friendly and lower-cost process to produce graphite anode material, as it is transitioned into commercial production. Future work will therefore focus on future cost reductions and process improvements. The reviewer found that to that end, the future work is well oriented to the remaining challenges and are relevant to the project goals and the goals of VTO in general to reduce the cost of Li-ion batteries for EVs.

Reviewer 3:

The reviewer remarked that Coulometrics indicates additional work will focus on future cost reductions, but it is unclear to what degree Objective #5's note on fabricating and testing 1000 mAh pouch cells for gassing rate evaluation.

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

Reviewer 1:

The reviewer detailed that for a widespread use of EVs, batteries with higher energy and lower cost than the current Li-ion batteries and reduced charging time are needed. New approaches to reduce the material costs are desired to meet DOE's cost targets, which this project has been addressing.

Reviewer 2:

The reviewer pointed out that graphite has been largely ignored in terms of battery study. The project is timely and of great importance to develop low-cost, high-performance batteries.

Reviewer 3:

The reviewer said this project addresses aspects of cell cost and performance via graphite enhancement.

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 materials processing as well as cell fabrication and testing seem well within the team's capability to complete the project by July 30, 2019.

Reviewer 2:

The reviewer said that resources are appropriate for the scope of the project

Reviewer 3:

The reviewer commented the project has used all available resources that ensure the success of the project.

Presentation Number: bat400
Presentation Title: Novel Liquid/Oligomer Hybrid Electrolyte with High Lithium-Ion Transference Number (Hi-LiT) for Extreme Fast Charging
Principal Investigator: Zhijia Du (Oak Ridge National Laboratory)

Presenter

Zhijia Du, Oak Ridge National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

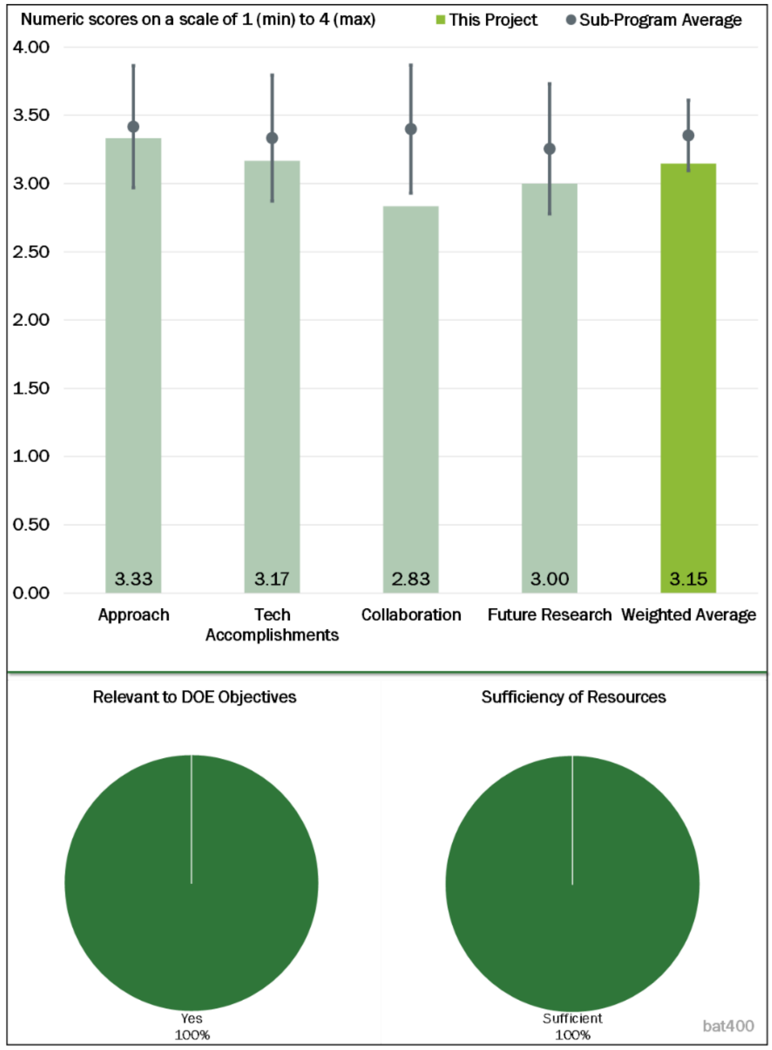

Figure 2-76 – Presentation Number: bat400 Presentation Title: Novel Liquid/Oligomer Hybrid Electrolyte with High Lithium-Ion Transference Number (Hi-LiT) for Extreme Fast Charging Principal Investigator: Zhijia Du (Oak Ridge National Laboratory)

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 said that the approach using liquid/oligomer hybrid electrolyte is novel and of great interest. The reviewer pointed out that the team consists of ORNL, University of Alabama-Huntsville, Virginia Tech, and Purdue. The experimentation was well designed and the results are solid and useful.

Reviewer 2:

The reviewer detailed that the objective here is to develop new electrolytes with high-Li-ion transference to enable a rapid charge (6C) of Li-ion cell, without having the issue of Li plating and without any decrease in the charge capacity. Specifically, the goal is to increase t_{Li+} from 0.36 to 0.75, while maintaining a relatively high conductivity of 4-10 mS/cm. The reviewer noted the approach being adopted involves evaluating new Li-salt anion oligomers that might suppress anion mobility and increase Li-ion transference number and new co-solvents with lower viscosity and improved ionic conductivity. The reviewer said that between the two approaches, adding a new co-solvent looks more feasible and effective, as also shown by the data here. However, it should be ensured that the new co-solvent does not impact the high temperature calendar life or make the safety characteristics worse compared to the baseline systems. The reviewer pointed out that regarding the anion aligomers, the gain in the transference number may be overshadowed by the reduction in conductivity. Also, the aluminum passivation characteristics of the new salt may not be as efficient as with $LiPF_6$ and need to be verified. Further, according to the reviewer the (fast) charging characteristics may be governed more by the concentration gradients within solid electrolyte interface (SEI) and electrode than electrolyte. The reviewer remarked some basic studies are required to segregate these two effects. Good baseline pouch cell design was developed, which is essential for these studies. Additionally, some basic studies have been made on understanding the changes in cathode upon fast charge. The reviewer found that the project is well designed to address the fast charging issue of Li-ion cells and is consistent with the goals of DOE's VTO. The project is well integrated with the other VTO projects.

Reviewer 3:

The reviewer remarked that the presented technical approach provides a feasible path toward focused enhancement of potentially extreme fast-charging (XFC) capable electrolytes and demonstration of their performance for evaluation.

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 the project has accomplished the first two milestones and the results are promising. The project is on track and in good shape.

Reviewer 2:

The reviewer said that results to date identify technical efforts that show progress as well as efforts that provide key learnings to modify and down-select effective paths forward. The reviewer noted that successful synthesis and characterization of initial additive-enhanced electrolytes has been demonstrated.

Reviewer 3:

The reviewer said that reasonably good progress has been made overall. Specifically, the project screened out four different co-solvents with an EC:EMC blend, out of which two co-solvents seem to offer higher conductivity and better cycling performance with fast charging. Likewise, the project synthesized two oligomer-type Li salts, which show much lower conductivity than the baseline. The reviewer pointed out that a new salt has been identified (the reviewer was not sure what this is, LiX) which has higher conductivity and transfer number and will be promising for future studies, similar to the co-solvents. Interestingly, ex situ studies on the fast-charged cathode show unexpectedly higher Ni oxidation state. Finally, a good pouch cell design has been developed to study the fast charge effects, though specific energies of 200 Wh/kg or less are not that impressive for pouch cells. The reviewer found that overall, the progress achieved here is meaningful and relevant to DOE goals.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented the project has an excellent collaboration and the team consists of complementary expertise.

Reviewer 2:

The reviewer said that there are good on-going collaborations here within the DOE National Laboratories (Liu from ORNL) and with external university partners, Zhang (University of Alabama-Huntsville), Lin and Schulz from Virginia Tech., and Zhao (Purdue University).

Reviewer 3:

The reviewer remarked with a large list of collaborators, the respective contributions of each individual member toward the greater project goals are 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 remarked that remaining tasks for the program will leverage initial results in synthesizing electrolytes with the focus on tuning viscosity and conductivity greater than the previous trials.

Reviewer 2:
The reviewer said that proposed future research has been well planned. The team members jointly work on the objectives with the goal to achieve 10-minute charge through liquid/oligomer hybrid electrolyte. The project may explore atomistic/MD simulations to understand the mechanisms that should in turn help seek alternative hybrid electrolytes.

Reviewer 3:
The reviewer said that being a new project, a few challenges still remain, i.e., to understand the fast-charge effects and to develop electrolytes that enable such fast-charging without Li plating and loss of performance (specific energy and cycle life). The reviewer said that the proposed studies of continued evaluation of more co-solvents and new Li oligomer salts with lower viscosity and higher conductivity and anion receptors and the post-mortem studies of Li-ion cells upon fast charge cycling are relevant. The reviewer referenced a prior comment, and said that it needs to be clearly established if the electrolyte properties or the SEI characteristics are governing the fast-charge behavior. The reviewer remarked more emphasis should be on the two solvents that showed promise, to ensure that they do not compromise other performance characteristics of baseline Li-ion cells.

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

Reviewer 1:
The reviewer remarked that the project addresses the urgent need for fast-charging through a hybrid electrolyte and supports DOE objectives.

Reviewer 2:
The reviewer said that for a widespread use of EVs, batteries with higher energy and lower cost than the current Li-ion batteries and reduced charging time (15 minutes or less) are needed. New electrolytes with improved bulk and interfacial properties are desired to meet the fast-charge goals of DOE, which this project has been addressing.

Reviewer 3:
The reviewer commented this program addresses DOE battery electric vehicle (BEV) cell performance and fast-charge specification in the enhancement of electrolyte characteristics.

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 scope of the project.

Reviewer 2:
The reviewer commented that partners in the program should have little issue in leveraging their collective resources to advance the state of the art in a feasible technical approach for XFC-capable electrolyte development.

Reviewer 3:

The reviewer remarked the team has used resources available at the National Laboratory and universities. The reviewer suggested that the project perform atomistic/MD simulations to understand the mechanisms of hybrid electrolytes.

Presentation Number: bat401
Presentation Title: Advanced Electrolytes for Extreme Fast Charging
Principal Investigator: William Chueh (Stanford University)

Presenter

William Chueh, Stanford University

Reviewer Sample Size

A total of four reviewers evaluated this project.

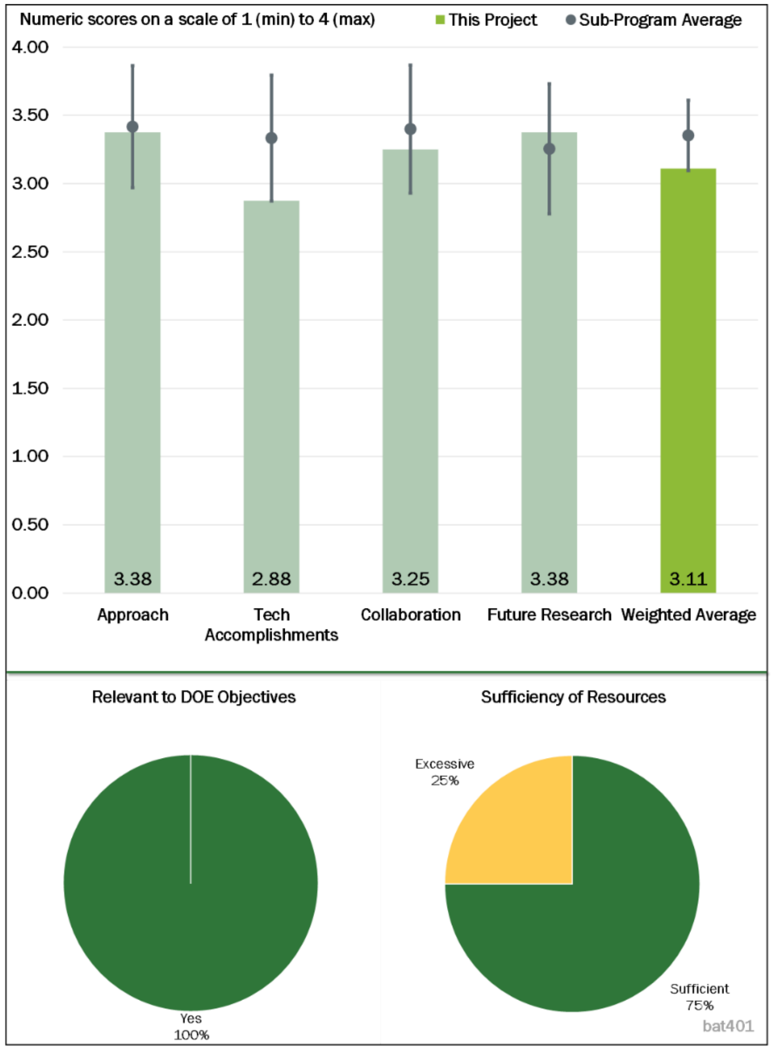

Figure 2-77 – Presentation Number: bat401 Presentation Title: Advanced Electrolytes for Extreme Fast Charging Principal Investigator: William Chueh (Stanford University)

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 found that the approach is novel and of great interest. The designed new electrolyte has shown excellent performance, and the team consists of researchers with complementary expertise.

Reviewer 2:

The reviewer detailed that this project is focusing on developing advanced electrolyte and charging method to enable battery fast-charging with thick graphite anode. The reviewer said that this approach is interesting. It is unclear if the approach can help solves the Li plating problems associated with low Li diffusion within graphite particle and graphite morphology change.

Reviewer 3:

The reviewer said that the presented approach addresses the technical aspects of electrolyte enhancement for XFC challenges as well as the design and characterization thereof.

Reviewer 4:

The reviewer detailed that the objective here is developing an advanced electrolyte for commercial graphite anodes to enable XFC. The approach involves optimizing the charging protocol, and more importantly understanding the impact of XFC on the battery components, and utilizing in situ X-ray and ex situ cryo-EM characterizations of full cells to understand and possibly control Li plating/dead Li formation in full cells during cycling. There is more emphasis here on understanding the nature of Li plating using the in-operando techniques, which is also the novelty here, than to control it via modification of the electrolyte. The reviewer pointed out that the electrolyte is no doubt a critical component to dictate the bulk conductivity, but also the interfacial properties (SEI characteristics), which are often more dominant at fast charge rates or low temperatures. There are other cell design aspects, e.g., cathode kinetics, ratio of negative to positive electrodes

(N/P ratio), electrode loadings etc., that play a crucial role as well. The reviewer said that not many details are provided here on the electrolyte development, except that it is has low-viscosity and high salt content. One likely casualty with the low-viscosity electrolyte would be its high temperature resilience, affecting the high-temperature calendar and cycle life. The reviewer said that the in situ techniques no doubt help in understanding the nature of plated Li, but the question would be what the guidelines are for the electrolyte selection, either from a modeling perspective or for an experimental implementation to control "the dead Li." The reviewer found that overall, the project is well-designed and feasible to an insight on Li plating, and may be integrated with other efforts addressing this aspect broadly.

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 that the project has accomplished much in terms of milestones. The developed new electrolyte has demonstrated its potential for fast charging. The coupled experimentation and simulations help understand the mechanisms. The reviewer found that the project is on track and in good shape.

Reviewer 2:

The reviewer found that reasonably good progress has been made so far in this project. The project has developed a low-viscosity, high-conductivity electrolyte. Again, not many details are provided here, but the electrolytes will need to be compatible with the cathode, and have adequate high-temperature stability so that the high-temperature calendar and cycle life are not adversely affected. The reviewer pointed out that the decline in performance with higher anode loadings during cycling with high charge rates is nothing unknown or unexpected. X-ray diffraction microscopy on the single-layer pouch cells reveals Li plating. It seemed to the reviewer that the test cell, either single layer or multi-layer graphite/lithium cobalt oxide pouch cells planned later in the project, are not appropriate test vehicles to address the fast-charge issue, which may be affected by other components and cell design aspects than just electrolyte. The reviewer said it may be more useful to utilize the diagnostic techniques being developed here on "more complete" cells from an external vendor, with a baseline electrolyte and the high-conductivity electrolyte. The reviewer found that overall the project is well oriented towards the project and DOE goals.

Reviewer 3:

The reviewer noted that the team has demonstrated some preliminary results of 10C rate charging with lower active materials loading. The reviewer said that more effort may be needed to demonstrate the efforts on cells with thick electrode.

Reviewer 4:

The reviewer said that progress towards an advanced electrolyte has been made, but there is further work to be done with the program starting in first quarter 2019. The reviewer noted that initial X-ray characterization efforts show potential, but further effort is needed as higher Ah prototype cells are fabricated.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the project has an excellent collaboration (Stanford, Stanford Linear Accelerator Center [SLAC] National Accelerator Laboratory, SpectraPowerLLC, and Colorado School of Mines).

Reviewer 2:

The team consisted of an industry partner, university, and National Laboratory, and it seems to have a good collaboration among team members.

Reviewer 3:

The reviewer observed that there are useful on-going collaborations in this multiple-PI project with several researchers: Chueh, Toney, Cui, Kaschmitter, Weker, Kee from two universities and also external participants (SpectraPower) and consultants (Victor Koch and Covalent Associates).

Reviewer 4:

The reviewer pointed out that being early in the program, there is demonstrated collaboration between program partners, but coordination and contributions to technical progress should mutually grow to achieve program deliverables.

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 is adequate.

Reviewer 2:

The reviewer remarked the proposed future research is well planned and positioned to achieve 10-minute charging through the design of new electrolytes.

Reviewer 3:

The reviewer commented there plenty of activities remain in this program and the noted future work, aligned with the presented Gantt chart, puts this program on a feasible path forward.

Reviewer 4:

The reviewer detailed that the proposed future studies of continued optimization of electrolytes in terms of salt concentration, co-solvent, and additive package to achieve the targeted high conductivity, and charging protocol to increase charging capacity at 10 minutes to 80%, performing X-ray and electron characterizations to assess the effect of electrolyte on SEI thickness, and Li plating during extreme fast charging, are logical and consistent with project goals. The reviewer referenced a prior comment, and said it would be better to use "more appropriate and mature/representative" test cells from a cell manufacturer with the selected electrolyte for the in-operando studies.

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

Reviewer 1:

The reviewer commented battery fast-charging is addressed by this project and new electrolyte design may help to meet the goal.

Reviewer 2:

The reviewer remarked that the program addresses aspects of XFC enabling technologies in the advancement of a high conductivity electrolyte.

Reviewer 3:

The reviewer said that for a widespread use of EVs, batteries with higher energy and lower cost than the current Li-ion batteries and reduced charging time (15 minutes or less) are needed. Fast recharge is problematic, because it leads to Li plating, which may adversely affect the safety and reliability of the cell. The reviewer pointed out that it is crucial to understand the nature of plated Li and to control it via modifying the cell components (electrolyte in this case) during fast charge and meet the goals of DOE, which this project has been addressing.

Reviewer 4:

The reviewer said the project addresses the urgent need for fast charging. The researchers from university, National Laboratory, and industry are teamed up to design new electrolytes with the goal to achieve DOE's targets.

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 used resources at university, National Laboratory, and industry, which are sufficient to achieve the milestones in a timely manner.

Reviewer 2:

The reviewer commented no indication that new resources are needed for this project.

Reviewer 3:

The reviewer stated that resources of the collaborative team align with the program's approach.

Reviewer 4:

The reviewer said that resources are much in excess for the scope and progress of the project.

Presentation Number: bat407
Presentation Title: Understanding and Modifying Cathode/Electrolyte Interfaces
Principal Investigator: Jie Xiao (Pacific Northwest National Laboratory)

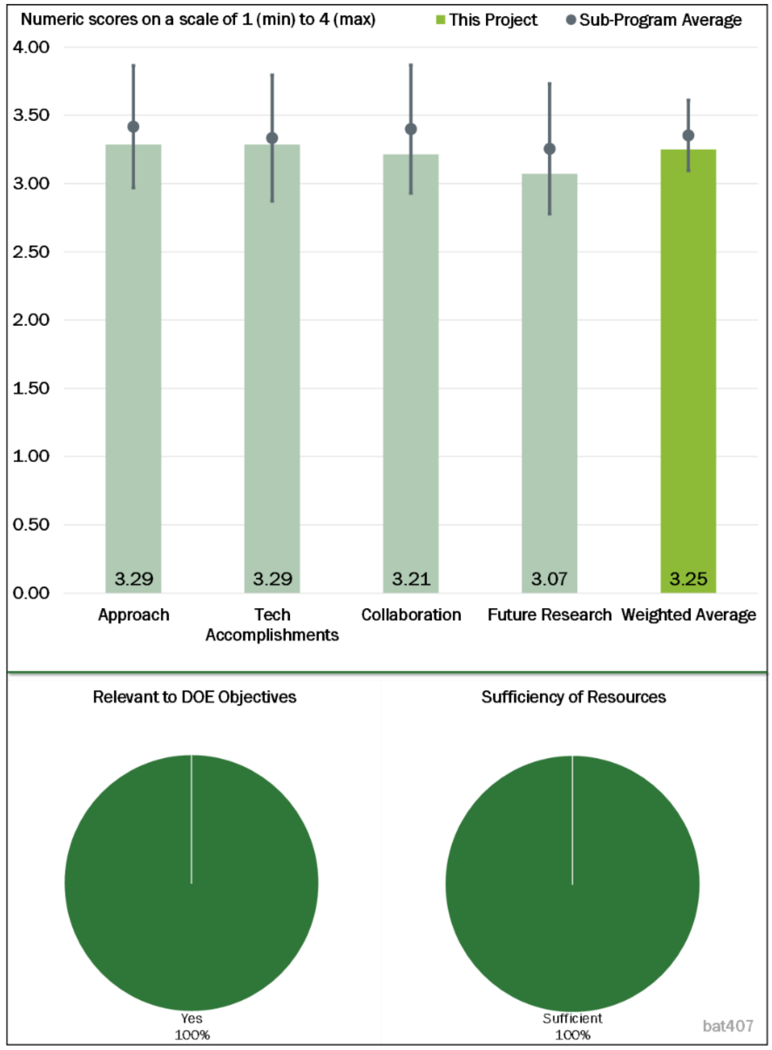

Figure 2-78 – Presentation Number: bat407 Presentation Title: Understanding and Modifying Cathode/Electrolyte Interfaces Principal Investigator: Jie Xiao (Pacific Northwest National Laboratory)

Presenter
Jie Xiao, Pacific Northwest National Laboratory

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

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

Reviewer 1:
The reviewer remarked the project adopts a synthesis approach to develop single-crystalline and polycrystalline morphologies for Ni-rich and low-Co cathodes and with a focus on thick electrodes.

Reviewer 2:
The reviewer said that the project is deliberately changing the surface area of the cathode material from single crystals to aggregates of small particles. The difference in surface are will enable assessment of the impact of the cathode-electrolyte interface (CEI) on the stability of the system.

Reviewer 3:
The reviewer said that the project targets barriers of low energy and high cost of batteries by seeking to employ materials with low cobalt (Co) content, and evaluating the possibility of increasing particle size to increase density. The approach of seeking high nickel (Ni) contents has an established track record and follows the trends in the field. The reviewer was less clear that the known critical issues with this approach are being tackled.

The reviewer remarked to further increase density and relate lab-scale electrode performance to the cell level, the project focuses on fabricating thick electrodes as objects of study. The combination of thickness and single crystalline microparticles produced incremental gains in electrode loading without compromising performance, which is a very welcome development.

Reviewer 4:

The reviewer said that while the goals of the project include demonstrating high-capacity, low- or no-Co cathode materials, the project is part of the Frontier Science element of the VTO portfolio on batteries which has a focus on characterizing and controlling the cathode-electrolyte interface. Therefore, it seems logical that the approach should focus more on the cathode-interface (characterization and control) than on morphology control during synthesis (poly crystalline versus single crystalline). The reviewer said that while the latter may demonstrate progress towards low- or no-Co materials with high capacity, this approach is largely centered on eliminating or minimizing the cathode-electrolyte interface. While that is a form of "control," it does little to understand and characterize the interface. The reviewer remarked that the work with Al doping to stabilize the interface is better aligned with the Frontier Science topic that the project is supposed to address. The team has an outstanding suite of advanced characterization techniques available to it (in addition to the synthetic capabilities that have been demonstrated in the early part of the project), and should be able to devote more of the project's approach to characterization of the interface as the project proceeds.

Reviewer 5:

The reviewer remarked the approach to the technical work is solid and backed up by good characterization; however, the project lacks substantial novelty. The reviewer cited as an example, single crystal nickel manganese cobalt (NMC) materials are already being commercialized, even if they are difficult to purchase. Also doping of NMCs, particularly with aluminum (Al), has been explored in other VTO projects previously at Argonne National Laboratory. The reviewer said that the focus on doped single crystal NMCs is somewhat new, but not revolutionary.

Reviewer 6:

The reviewer noted that single crystal NMC seems interesting. However, this approach is not so novel. The reviewer said that a lot of teams have been successful in synthesizing this kind of material.

Reviewer 7:

The reviewer remarked that the approach in this project explores a possibility to maximize cell-level energy for Li-ion batteries via synthesis of Ni-rich and low-Co cathode materials with polycrystalline and single crystal morphologies and to tailor cathode/electrolyte interface for extended long-term cycling and reduced gas evolution via Al doping strategy possibly leading to modified surface properties and improved cycling stability. Developed approaches will be used and tested for thick cathodes. The reviewer noted that single crystalline cathode materials are believed to advantageous for Li-ion batteries as they can result in reduced gas evolution, reduced sensitivity to moisture, lower surface area, and increased tap density. However, single crystalline materials generally exhibit lower contact area between electrode and electrolyte and increased diffusion distances, as compared to the polycrystalline materials, which usually results in lower specific capacities and reduced rate performance. The reviewer said that the presenter failed to explained how these challenges are proposed to be overcome.

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 despite being started only a few months ago, the project has achieved several key milestones in the synthesis of morphology-controlled cathode materials and Al-doped cathode materials. The project appears to be off to a fast start. The reviewer noted that characterization data have already been obtained, and it is clear that the project is making real progress in the initial phase, and that the pace of activities is excellent so far.

Reviewer 2:
The reviewer said that the project is in its first few months from inception, and pointed out that the team has already demonstrated synthesis and electrochemical performance of $LiNi_{0.76}Mn_{0.14}Co_{0.1}O^2$ (NMC76)-based thick cathodes with both single crystalline and polycrystalline morphologies.

Reviewer 3:
The reviewer noted that this is a new project, so the need for ramp-up is evident in the progress. Because the approaches followed are rather classical, many of the results conform to very well-established trends in the field, so the level of new insight is only moderate. The reviewer pointed out that the most intriguing aspects came from the results with single crystalline particles, which were surprisingly close to polycrystalline counterparts, especially considering the higher loadings. It seemed to offer good prospects to meet the goals in terms of performance indicators.

Reviewer 4:
The reviewer said that progress has been made in the synthesis of the materials. Initial electrochemistry has also been obtained. The reviewer found that progress is fully reasonable given the short time that the project has been underway.

Reviewer 5:
The reviewer said that this project was very recently started, yet there has been fairly good progress in the initial months. The reviewer detailed that polycrystalline and single crystal NMC cathode materials have been synthesized and meet the capacity criteria set in the project plan. Electrodes have been generated which appear adequate. Researchers should be commended for selecting and achieving an aggressive electrode formulation (low carbon and low binder with appropriate press densities) which is relevant to automotive applications. The reviewer noted that while an NMC with 76% Ni is not particularly aggressive, it provides a reasonable model system for studying cathode longevity and gassing at the particle and electrode level. The reviewer pointed out that while investigating the impact of doping on single crystal NMCs, it would be valuable to include dopants other than Al for a better understanding of how dopants suppress reactions with the electrolyte or phase changes in the particle.

Reviewer 6:
The reviewer said it is not clear whether single crystal NMC can perform better than the polycrystalline one based on the data presented. The capacity gap is very big now.

Reviewer 7:
The reviewer remarked that the project started in October 2018; this is the first project period. During this initial stage of research, the focus was on developing synthesis parameters for Ni-rich and low-Co NMC polycrystalline and single crystal cathode materials and incorporate synthesized materials into thick electrodes. The reviewer detailed that progress includes single crystalline and polycrystalline NMC76 materials have been synthesized with similar size of particles (3-4 um), while polycrystalline material consists of nano-sized primary grains; it was found that the polycrystalline material initially shows high specific capacity than the single crystalline material; and porosity of the thick electrodes is slightly high in case of the polycrystalline materials (65% vs 62%).

The reviewer posed multiple questions. The reviewer asked why lower surface area enabled by single crystalline materials is of interest, and pointed out that lower surface area usually leads to lower contact area with electrolyte and poorer rate capability. The reviewer also noted that improvement in electrochemical performance of single crystalline cathodes is proposed through optimization of the synthesis process, however no details are provided. The reviewer asked how synthesis process will be modified to improve performance, and additionally how Al doping in single crystalline materials will be achieved. The reviewer noted that one of the advantages of single crystalline particles is that only certain crystallographic planes are exposed on the surface. This opens an opportunity for surface engineering via targeted modification of the surface-exposed crystallographic planes. The reviewer asked if there are any experiments planned to explore surface engineering approach for single-crystalline electrodes. Finally, the reviewer asked will the whole project be focused on investigating NMC76, or will other cathode chemical compositions will be explored, and why.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that it is very early still, but the level of collaboration appears to be excellent and the major reason for the fast start to the project. This team at Pacific Northwest National Laboratory (PNNL) has a history of excellent collaboration and the early trend is consistent with past performance.

Reviewer 2:

The reviewer observed that the team has a planned collaboration with Brookhaven National Laboratory (BNL) for X-ray diffraction (XRD) characterization and structural analysis.

Reviewer 3:

The reviewer noted that the project just started so collaboration with partners is at a preliminary level.

Reviewer 4:

The reviewer commented that the team is located at PNNL, and currently collaborates only with researchers at BNL on XRD characterization and structural analysis. The team will seek for more collaborations based on the progress and needs of the project.

Reviewer 5:

The reviewer said that this program is a focused program, thus there are not many partners involved. The current focus on synthesis and initial electrochemistry is appropriate.

Reviewer 6:

The reviewer pointed out that most of the data seemed to come from the PIs group, with the exception of routine transmission electron microscopy (TEM). It underutilizes the extensive skills of Chongmin Wang at PNNL. The reviewer was unclear why there is a need to incorporate BNL for XRD analysis, given that no specialty measurements are planned.

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 the project has a clearly outlined plan for improvements with single crystalline morphologies and assessing the efficacy of doping/coating for thick electrodes.

Reviewer 2:

The reviewer remarked that the proposed future work is of interest. Addressing all of the questions posed is ambitious, but will provide useful insight for the program.

Reviewer 3:

The reviewer said that no decision points or alternate development pathways were presented. The proposed future research is sensible, albeit vague at times, and again follows rather established pathways. The reviewer remarked that the efforts to boost the performance of thick electrodes with single crystalline particles should be emphasized.

Reviewer 4:

The reviewer said that the proposed future work is too vague to guide further study. No detail is given on new tools or techniques that will be used to investigate failure mechanisms or improve performance. It is difficult to determine what hypothesis is being studied here. It is desirable to include rate capability as a criterion for performance evaluation, especially with single crystal particles and dense electrodes. The reviewer remarked that researchers may also consider adding one or two other cathode compositions (i.e., higher Ni % or nickel cobalt aluminum oxide [NCA]).

Reviewer 5:

The reviewer found that the proposed future work is logical and consistent (mostly) with project goals. As noted above, it may be desirable to spend less effort trying to make single crystal material work as well as polycrystalline material and focus more effort on interfacial dynamics/degradation and subsequent control. The reviewer noted that the latter will be applicable to virtually all cathode materials above 4.3 volt (V)—not specific to one material. The reviewer found that additionally, the proposed work "Investigate the failure mechanism of Ni-rich and low-Co cathodes at relevant conditions, e.g., mass loading, full cell, electrolyte content" needs some more definition. The reviewer inquired going forward what specifically are the most important characterizations to do first. There have been lots of research groups looking at cathode and cathode-electrolyte instabilities at high voltage with limited success so far (hence the emphasis here in Frontier Science). The reviewer asked what the most important things to do next are.

Reviewer 6:

The reviewer pointed out that the future work will be focused on modifying synthesis parameters for single crystal NMC76 cathode to achieve improved electrochemical performance and enable Al doping. The failure mechanism of Ni-rich and Co-low cathodes will be investigated. The reviewer noted that comparison of the single crystal and polycrystalline NMC76 in terms of their gas generation will be performed. However, the specific strategies that will be taken to improve performance of the single crystalline electrodes were not revealed in either slides or at the poster discussion.

Reviewer 7:

The reviewer is not convinced a better performing single crystal material can be achieved by optimization of synthesis, which was not disclosed.

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

Reviewer 1:

The reviewer remarked that the project is aligned with the goal toward accelerated development of next-generation Li-ion battery technology.

Reviewer 2:

The reviewer pointed out that the alignment between project objectives and DOE goals is very strong. If successful, the project will have significant impact on DOE's ability to reach key milestones on their roadmap for energy storage—particularly for batteries with high-capacity, low- or no-Co cathode materials.

Reviewer 3:

The reviewer noted that the stability of the cathode surface is an important aspect of advancing next-generation battery science.

Reviewer 4:

The reviewer said that this project seeks to increase the energy density of batteries while lowering cost. It squarely targets a critical barrier in battery technology.

Reviewer 5:
The reviewer remarked that this project should address the need to understand decomposition mechanistically at cathode-electrolyte interfaces with new NMCs. Impacts include better design of cathodes to promote safety and cycle life.

Reviewer 6:
The reviewer noted that due to some advantages that can be achieved through utilization of single crystal particles as active material in cathode fabrications, this research can contribute to DOE's efforts in developing Li-ion batteries with high energy density. According to the reviewer, the power density, as the team admits, will most likely suffer due to the lower surface area and longer diffusion distances characteristic of single crystals as compared to the polycrystalline materials.

Reviewer 7:
The reviewer indicated performance and cost of battery materials.

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

Reviewer 1:
The reviewer found that the resources for this project are sufficient.

Reviewer 2:
The reviewer said that while still early, the resources allocated to the project appear to be sufficient to achieve the milestones as planned. The reviewer pointed out that as in any R&D project, there are far more opportunities for experimentation than there is budget, so the team will have to be strategic in their selections. But the project appears to be largely on track at this early point.

Reviewer 3:
The reviewer commented the team has adequate resources needed for successful accomplishments as planned.

Reviewer 4:
The reviewer said that resources available for the team are adequate.

Reviewer 5:
The reviewer remarked resources are sufficient for the current phase of the research program.

Reviewer 6:
The reviewer had no comment.

Reviewer 7:
This reviewer stated none.

Presentation Number: bat408
Presentation Title: Interfacial Studies of Emerging Cathode Materials
Principal Investigator: Marca Doeff (Lawrence Berkeley National Laboratory)

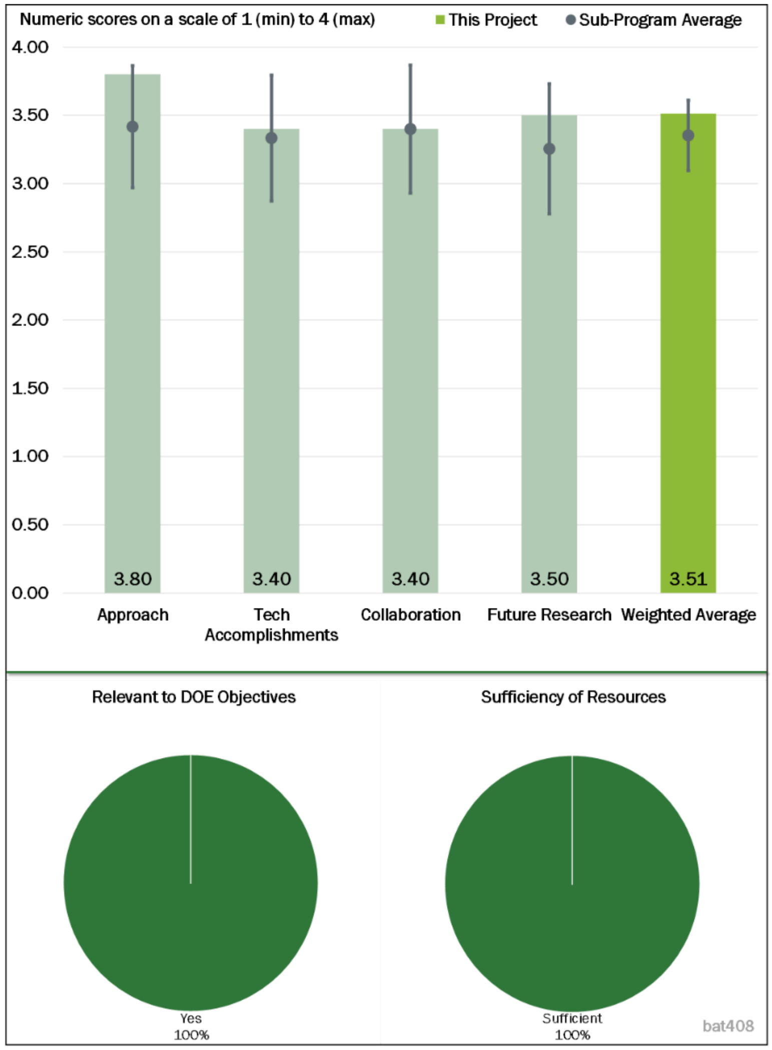

Figure 2-79 – Presentation Number: bat408 Presentation Title: Interfacial Studies of Emerging Cathode Materials Principal Investigator: Marca Doeff (Lawrence Berkeley National Laboratory)

Presenter

Marca Doeff, 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 the approach to the technical work is solid and backed up by excellent synchrotron-based characterization techniques. The focus of this project on providing a fundamental material stability basis for cathode-electrolyte interface decomposition as well as at the bulk particle level is highly valuable for cathode design. The reviewer said that the approach of partnering in situ and ex situ experiments is reasonable giving the limitations of each.

Reviewer 2:

The reviewer pointed out the project has not really begun because the team was granted permission from DOE to complete previous work on Ni-rich NMC811 and its thermal behavior. Nevertheless, the approach planned for the new work on cathode materials which display oxygen (O_2) redox (some model materials were chosen that work okay and some do not) will be similar, and the general approach to studying the complex and coupled dynamics of cathode materials is excellent. The reviewer noted that the approach is very comprehensive but strategic—including techniques that probe various depths and time scales, as well as both operando and ex situ characterizations. The reviewer found that all of this work seems well balanced and thoughtful. In short, it is clear that strategic decisions are being made about what makes sense to characterize and what techniques should be used—rather than just trying to run every experiment/characterization possible regardless of potential impact on the project's goals.

Reviewer 3:

The reviewer remarked to apply various techniques to characterize the materials and interfaces is exciting. Fruitful results are expected.

Reviewer 4:

The reviewer said that the approach is a fundamentally driven science strategy that includes a suite of bulk and surface-sensitive synchrotron techniques to study interfacial reactivity and stability of emerging cathode materials (with high O-redox capacity).

Reviewer 5:

The reviewer said that this project is transitioning from the study of thermal runaway in layered materials to the elucidation of interfacial phenomena unique to so-called "O redox materials." Both families present unique challenges, but they are the leading and emerging choices, respectively, to address barriers of energy and safety underpinned by the cathode. Therefore, according to the reviewer both efforts are extremely worthwhile.

The reviewer said that the project critically relies on a vast suite of modern synchrotron methods. This approach will surely provide significantly unique and novel insight. However, per the reviewer, a combination of many sophisticated experimental tools with the study of several "O redox" materials presents the risk of spreading resources thin. The reviewer said that the PI should consider perhaps a narrower focus to materials with true prospects of commercialization, such as those based on manganese (Mn) or Fe-Sb, and leave curiosities with Ruthenia (Ru) or iridium (Ir) to more academic endeavors.

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 the PI and team have made fundamental contributions to understanding the interfacial reactivity of Ni-rich (concluding part of the earlier project) cathodes and are off to a good start on the proposed O-redox cathode materials.

Reviewer 2:

The reviewer said that progress has been comprehensive, with a new sophisticated understanding of thermal runaway in NMCs at a local level. Progress toward the new project has been more modest in comparison, but still in line with the proposed milestones for fiscal year (FY) 2019 quarter 2. The reviewer said while reasonable based on the refocusing of the effort, progress should be pushed forward aggressively.

Reviewer 3:

The reviewer pointed out that this project was very recently started, yet there has been very good progress toward the goals. The initial project intended to focus on titanium (Ti) substituted NMC 811, but having now completed work on NMC 811, it will be transitioned to emerging oxygen-redox cathodes. The reviewer found that despite the no-go decision, the work on NMC 811 is excellent and should be valuable to future research on high-Ni NMCs. In fact, it would be possible and still valuable to continue work on high-Ni NMCs and NCAs because of their relevance to commercialization. Regardless, the findings concerning reduction and oxidation of surface versus bulk species at various levels of cathode lithiation help to explain the decomposition of these materials at higher temperatures. Such insights are only available via the combination of precise techniques used in this type of project.

Reviewer 4:

The reviewer said that the team made "excellent" progress in closing out the previous work on the complex thermal behavior of Ni-rich NMC811. The results are very nice and will have impact on battery technology. The reviewer noted that the level of detail in the characterizations of NMC811 was excellent. Unfortunately, completing this work delayed the start of the new work on cathode materials exhibiting oxygen redox processes. So, there is little if anything accomplished for the new start—other than to select the model materials for study. The reviewer commented hopefully, the team will be able to use its experience and extensive capabilities in battery materials to realize a very fast start to the new work and will be able to "catch up" over the next project year. But the closeout of the NMC811 work was done very well.

Reviewer 5:
The reviewer pointed out the project just started.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer remarked collaboration with SSRL and also with the industrial and academic partners is noteworthy.

Reviewer 2:
The reviewer found that collaboration across partner teams appears good.

Reviewer 3:
The reviewer noted that the PI works closely with synchrotron scientists at SSRL, which provides critical expertise to complete comprehensive studies. The role of Virginia Tech after the refocusing of the project was unclear.

Reviewer 4:
The reviewer stated the pace of activities and complexity of the work clearly benefits from excellent coordination and collaboration across the team. This collaborative approach will be necessary for the team to make a fast start on the new project and recover the schedule lost due to finishing the NMC811 work.

Reviewer 5:
The reviewer remarked the role of each team is 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 said the project has outlined a clear plan and pathway for synthesis and down-selecting O-redox cathode materials followed by detailed electrochemical analysis and synchrotron-based studies.

Reviewer 2:
The reviewer remarked this project has incorporated effective go/no-go decision points, and it appears that multiple development pathways are considered. The reviewer commented that future research covers a critical stepping stone for the applicability of the so-called "O_2 redox" concept, and the plan of action is ideally suited for this purpose.

Reviewer 3:
The reviewer remarked the future work is described at a very high and generalized level—so a little bit more detail overall would have been helpful. The complexity of oxygen redox coupled to irreversible oxygen loss might need additional characterization techniques, so some additional details about what the immediate challenges for materials characterization that needs to be tackled first would have been helpful. However, according to the reviewer, assuming that project follows the same basic pathway that the team followed in the NMC811 work, the project will be fine.

Reviewer 4:
The reviewer remarked relevant with the objectives.

Reviewer 5:

The reviewer remarked being that the project recently transitioned to focusing on a new material set of oxygen-redox cathodes, more precise plans would be helpful. A number of new materials have been selected, but it is unknown if these are "model systems" for studying oxygen redox or instead, relevant commercially. The reviewer noted that the techniques used in the earlier part of the project would certainly be applicable to the new work, but there are a number of issues, including radical phase changes, that could complicate a study on this new class. The reviewer stated being that this new focus will use lab synthesized material, it would be useful to identify commercial pathways for this type of material by talking with material suppliers (e.g., BASF).

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

Reviewer 1:

The reviewer pointed out that as the need for higher energy batteries drives the voltage at the cathode well above 4.3V and higher, the issue of oxygen redox is becoming increasingly important. The reversibility of oxygen redox and ultimately the limits that it puts on the lifetime for high energy systems are key issues that need to be understood for DOE to reach milestones on its technology roadmap for energy storage/batteries. Thus, the alignment of this project is very good with DOE objectives.

Reviewer 2:

The reviewer remarked this project targets critical new knowledge with a family of cathodes for high-energy density batteries. It fits very well with current DOE objectives.

Reviewer 3:

The reviewer stated this project addresses the need to understand cathode decomposition mechanistically. Impacts include better design of cathodes to promote safety and cycle life.

Reviewer 4:

The reviewer found that the project is aligned with the goal to contribute to the development of emerging cathode materials with high O_2-redox capacity toward achieving enhanced safety and cyclability.

Reviewer 5:

The reviewer noted that understanding the reaction mechanisms and relationship between the material properties and performance is critical to design better battery materials.

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

Reviewer 1:

The reviewer said resources for this project are sufficient.

Reviewer 2:

The reviewer remarked the project is just now starting, but the resources allocated appear to be sufficient to achieve the stated milestones by the end of the project. Leveraging of the National Laboratory user facilities via user proposals certainly helps provide the project valuable additional resources.

Reviewer 3:

The reviewer observed that the team has adequate access to the state-of-the-art synchrotron facilities.

Reviewer 4:

The reviewer had no comments.

Presentation Number: bat409
Presentation Title: Molecular-Level Understanding of Cathode/Electrolyte Interfaces
Principal Investigator: Mike Toney (SLAC National Accelerator Laboratory)

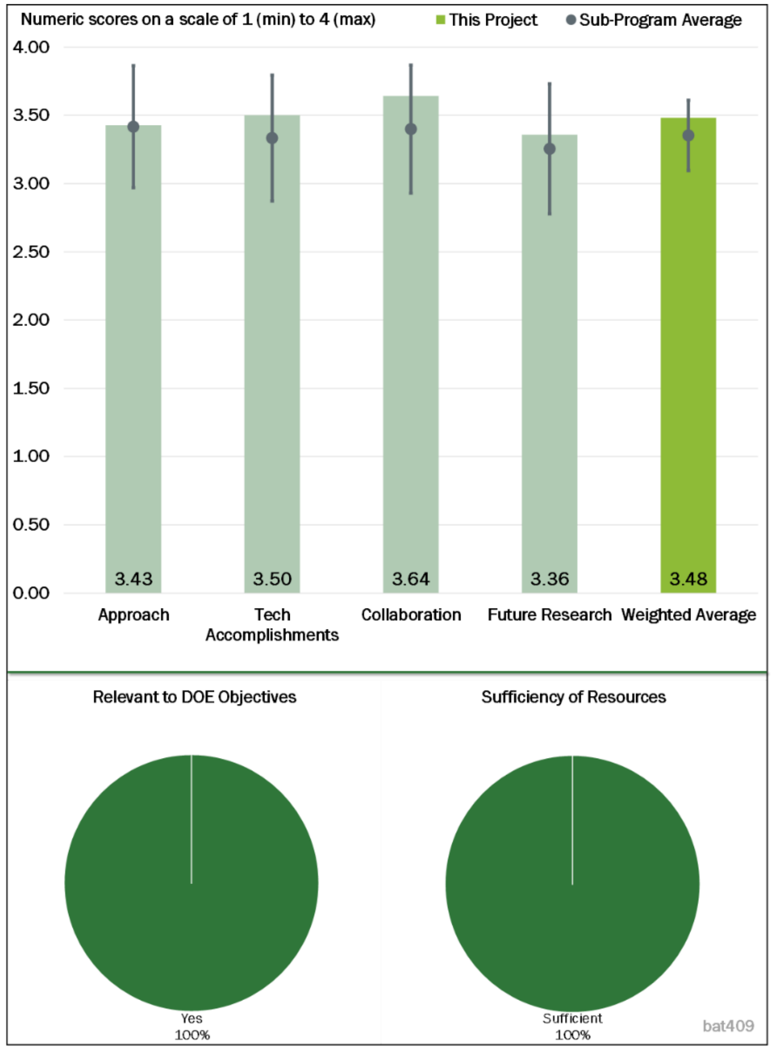

Figure 2-80 – Presentation Number: bat409 Presentation Title: Molecular-Level Understanding of Cathode/Electrolyte Interfaces Principal Investigator: Mike Toney (SLAC National Accelerator Laboratory)

Presenter

Mike Toney, SLAC National Accelerator Laboratory

Reviewer Sample Size

A total of seven reviewers evaluated this project.

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

Reviewer 1:

The reviewer detailed the approach includes a synergistic strategy combining molecular-scale MD and density functional theory [DF])) modeling along with X-ray-based characterization and electrochemical tests to study the complex processes in the CEI for high-voltage transition metal oxide (TMO) cathodes.

Reviewer 2:

The reviewer remarked the combination of experiment and theory is a good approach to probe this issue. The study is based on model systems in thin form format to facilitate the experimental characterization.

Reviewer 3:

The approach in this project involves combined computational and experimental approaches to understand processes that control CEI formation in high-voltage Li-ion batteries and develop strategies that enable stabilization of CEI under strongly oxidizing high-voltage conditions. Computational methods include molecular-scale MD simulations and DFT calculation. Experimental techniques include X-ray surface scattering, X-ray spectroscopy, and electrochemical characterization. Electrolyte materials range from conventional carbonate-based electrolytes to high-voltage electrolytes. TMO electrodes are synthesized in the form of particles and thin films grown by pulsed laser deposition (PLD).

Reviewer 4:

The reviewer detailed that this project focuses on the fundamental understanding of the interface between a model cathode and conventional Li-ion battery electrolytes. This is a perennially important problem that affects both energy density and lifetime. The reviewer said the project intends to relate observations from these model systems to real electrodes, but the approach was less clear on this aspect.

Reviewer 5:

The reviewer remarked the approach to the technical work is interesting, if not particularly novel. The goal of achieving a better mechanistic understanding of electrolyte impacts with high voltage cathode surfaces is important, but there are some doubts about the current approach. The unification of experimental and computation work is key to proving value; however, the assumption that real cathode surfaces can be appropriately modeled and/or reproduced epitaxially has considerable risk. The reviewer pointed out that the PLD technique, for example, results in different surface terminations based on background gas composition and pressure, as well as substrate orientation, and thermal annealing. The identification of relevant surfaces from practical materials is also challenging as most cathode materials are polycrystalline.

Reviewer 6:

The reviewer noted that gaining a molecular level understanding of the structure, composition, and dynamics of the CEI—including the buried CEI—is certainly a difficult challenge, but the combination of modeling, precise synthesis, and advanced characterization that will be employed here is outstanding. Each element is well thought out and likely to contribute to an increased understanding and control of the CEI. The modeling approach is fairly routine and probably not high enough fidelity to be very predictive, but it should be effective in interpreting experimental data.

The reviewer said the operando and real-time X-ray surface scattering and spectroscopy experiments are difficult, but really the only way to effectively characterize the dynamics of an electrode-electrolyte interface. The reviewer remarked these advanced characterization techniques are essential to the approach. The reviewer said using thin films on a planar substrate as the model system is a reasonable approach, but given the different level of defects, stress states, perhaps different surface chemistry (crystalline faces, etc.), and of course surface curvature, this approach has some limitations in understanding the behavior of real cathode materials. But at the molecular scale, the thin film format is probably a valid model—the difference in thin film versus nanoparticle performance generally appears at the mesoscale and above. Finally, although CEI is far less studied that SEI, there are lots of data and many examples in the literature so far about what techniques work and what limitations there are with various modeling and experimental techniques for electrified solid-liquid interfaces. The reviewer said that hopefully some of that previous work will help prevent reinvention of the wheel in this project. Similarly, there are lots of data on thin film cathode synthesis for solid-state batteries that can be leveraged potentially for this project.

Reviewer 7:

The reviewer said this project mainly focuses on DFT and X-ray scattering study on the interfacial reaction of electrolyte/electrode. It is not clear to the reviewer how the molecular level understanding can be achieved by X-ray scattering.

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 even though the project just started, some results have been obtained in modeling.

Reviewer 2:

The reviewer remarked this newly started project is off to a good start and has prepared baseline electrolyte and first MD simulation of the proposed electrolyte-model oxide interface.

Reviewer 3:

The reviewer noted that this is a recently started program and progress is appropriate. The theory piece is currently running ahead of experiment, but that can be useful in helping to guide the experiment.

Reviewer 4:

The reviewer said that the project is very new and there has been little time for any real significant achievement, but the project appears to be off to a fast start and ready to hit its milestones by the end of the first year. The reviewer detailed that materials have been successfully synthesized, MD calculations on EC solvents are done, and the basic electrochemical characterization has been completed. Of course, the more difficult scattering and spectroscopy experiments are on the horizon, but the initial progress has been excellent. The reviewer said that the project is off to a fast start—maintaining this pace through the advanced characterization stage in 2020 will be critical for the project to reach its stated goals.

Reviewer 5:

The reviewer pointed out that this project started this year and already has both experimental and computational results to show, although the milestones for the initial period were not overly ambitious. On the flip side, it seems like progress toward the third milestone of the year may actually be ahead of schedule, which according to the reviewer is obviously welcome.

Reviewer 6:

The reviewer said that as the project has very recently started, there is limited progress to report. Some NMC 532 films have been produced and analyzed electrochemically, showing very different behavior based on processing conditions. The reviewer pointed out that while PLD is controllable, it is difficult to know which surfaces are relevant to real systems. Preliminary modeling work shows some success with EC electrolytes (not yet sulfolane), but the same challenge holds here for creating an appropriate surface.

Reviewer 7:

The reviewer remarked the project has started in January 2019; this is the first project period. Despite an initial stage of this project, some technical achievements have already been demonstrated. The reviewer detailed accomplishments. First, DFT calculations revealed the decomposition behavior of different solvents and salts on the surface of the model $LiNiO_2$ cathode. Effect of the salt concentration is investigated. It was found that all electrolytes under study undergo deprotonation. Second, PLD-synthesized NMC532 thin film electrode has been studied electrochemically in the purified highly-fluorinated and sulfolane-based electrolytes. The reviewer had no questions.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer commented that given the combined experimental/modeling approach, the coordination between team members is critical to the success of the project and has been excellent so far. It appears that the calculations from the Army Research Laboratory (ARL), synthesis from Lawrence Berkeley National Laboratory (LBNL), and electrochemical and materials characterization at SLAC are all in sync, and the collaboration is going extremely well so far. The reviewer had no concerns about the cooperation or level of collaboration.

Reviewer 2:

The reviewer pointed out that synergy among the multi-institutional teams is noteworthy.

Reviewer 3:

The reviewer found that this project leverages clear synergies between SSRL, LBNL and ARL. It is effective in this regard.

Reviewer 4:

The reviewer pointed out that the project team consists of researchers from the SLAC National Accelerator Laboratory, ARL, and LBNL and research is well coordinated by establishing clear roles for computational science experts and experimentalists in the team. The team members are experts in their respective fields.

Reviewer 5:
The reviewer said materials were supplied by collaborators.

Reviewer 6:
The reviewer found that collaboration among the team appears strong with specific players with defined roles.

Reviewer 7:
The reviewer remarked that as the project just started, collaboration between the partners 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 detailed that the team will study a PLD-grown NMC532 cathode with different electrolytes both computationally and experimentally. Most excitingly, the team will characterize CEI evolution using real-time X-ray surface scattering and spectroscopy studies.

Reviewer 2:
The reviewer said that this new project has a clearly laid out plan (fundamental characterization and theoretical/simulation studies) to understand the CEI.

Reviewer 3:
The reviewer referenced previous comments, and said that there is considerable risk in this project but the team has selected appropriate go/no-go decision points. Significant value can be added by in situ/operando measurements as proposed.

Reviewer 4:
The reviewer noted that the proposed future research very logically flows from the original objectives. The decision points were vague and did not identify alternative pathways. The reviewer pointed out that the risk of not succeeding in the growth of films with relevant electrochemical performance is not mitigated, as only one way forward is considered.

Reviewer 5:
The reviewer said that the project is just now getting going, but the future work planned (mostly advanced X-ray scattering and spectroscopy experiments) is appropriate, and the risk is manageable. These are not easy experiments —the frequent use of modeling will help in the interpretation of data. The reviewer noted that the most valuable work likely will be the future results from the fluorinated solvents and sulfolanes—so the team is encouraged to be strategic in the initial EC studies and not get bogged down in details that are not necessarily relevant to real-world cathodes.

Reviewer 6:
The reviewer commented future studies are relevant with the project objectives. Again, this reviewer is not very convinced that the molecular level understanding can be achieved by only simulation and X-ray scattering.

Reviewer 7:
The reviewer said the team has appropriately defined their future goals. The PLD film still needs optimization. This will enable testing with a variety of electrolytes. The reviewer said these studies can then run along with the X-ray studies of the surface films.

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

Reviewer 1:
The reviewer pointed out that cathode/electrolyte interfaces are key to batteries with both high energy and long lifetime. Both are desired goals of DOE.

Reviewer 2:
The reviewer said that the role of the CEI is important and gaining insight will advance the goals of the program.

Reviewer 3:
The reviewer said that the project is aligned with advancing the Li-ion battery technology with improved CEI stability of high-voltage TMO cathodes toward enhanced energy density and life.

Reviewer 4:
The reviewer commented that this project should address the need to understand decomposition mechanistically at CEI at high voltage using specifically designed electrolytes. Impacts include better design of interfaces to promote the safety and cycle life of cathodes.

Reviewer 5:
The reviewer detailed that as the voltage of the cathode increases below 4.3V to achieve higher capacities, the nature and dynamics of the CEI (which has largely been ignored below 4.3V) is becoming more important and one of the most important technological issues for rechargeable batteries (cathode structural and phase stability being another). Thus, according to the reviewer, this work is very timely and very well aligned with the DOE objectives on their roadmap for electrical energy storage for vehicle electrification.

Reviewer 6:
The reviewer said the research is relevant to the DOE efforts in developing Li-ion batteries with high energy density, and high power density. Specifically, this project addresses degradation of high-voltage TMO cathodes via understanding of the mechanisms and developing strategies to stabilize CEI.

Reviewer 7:
The reviewer remarked understanding the active material and electrolyte interaction.

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 resources for this project are sufficient.

Reviewer 2:
The reviewer pointed out that the project is just starting, but resources (including the leveraging of resources at the DOE National Laboratory user facilities via user proposals) seem sufficient and adequate to achieve the stated milestones. There are no concerns at this point.

Reviewer 3:
The reviewer said the team has adequate access to the required characterization/experimental and computational resources.

Reviewer 4:
The reviewer remarked the resources available for the team are adequate.

Reviewer 5:
The reviewer said that the resources appear sufficient.

Reviewer 6:
The reviewer had no comments.

Reviewer 7:
The reviewer noted that the project relies critically on success via the growth of thin films by PLD. Yet, the growth is carried out by LBNL, which is, by far, the most junior partner in the budget. The reviewer remarked the PI should ensure sufficient resources are allocated to this task, because it is a bottleneck in the project as defined.

Presentation Number: bat410
Presentation Title: Developing Scanning Electrochemical Microscopy (SECM) for Cathode Interfaces
Principal Investigator: Robert Tenent (National Renewable Energy Laboratory)

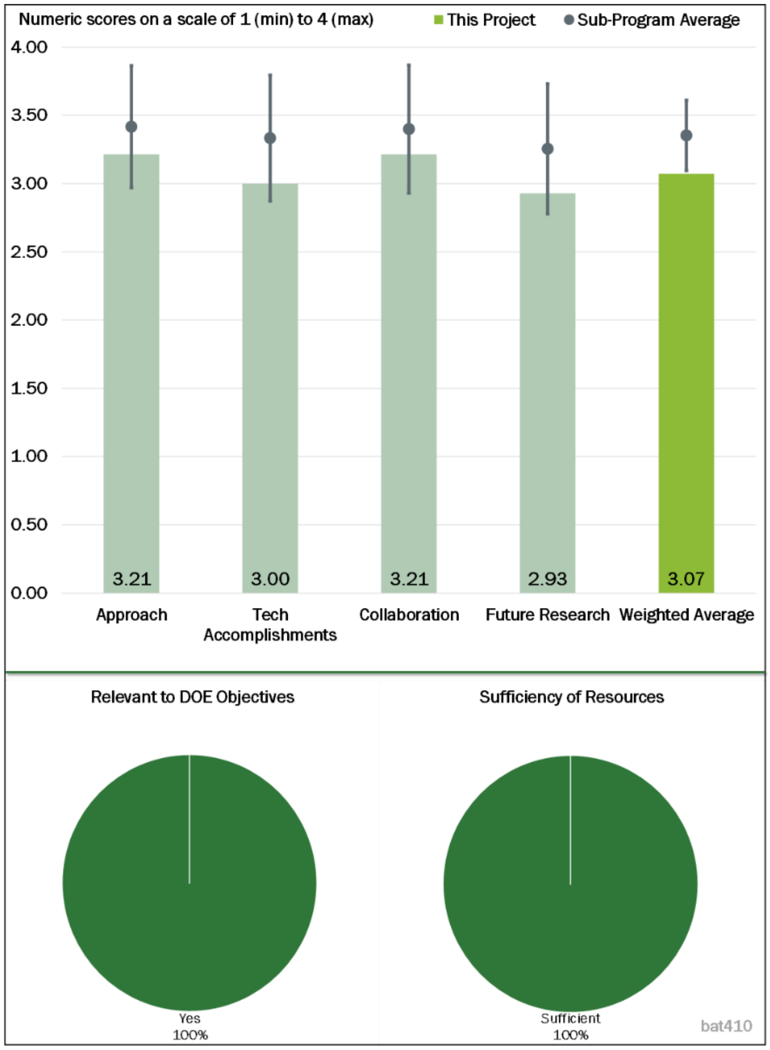

Figure 2-81 – Presentation Number: bat410 Presentation Title: Developing Scanning Electrochemical Microscopy (SECM) for Cathode Interfaces Principal Investigator: Robert Tenent (National Renewable Energy Laboratory)

Presenter

Robert Tenent, National Renewable Energy Laboratory

Reviewer Sample Size

A total of seven reviewers evaluated this project.

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

Reviewer 1:

The reviewer noted that the approach is valuable in probing surface phenomena.

Reviewer 2:

The reviewer noted that the approach relies on the scanning electrochemical microscopy (SECM)-based in situ technique to probe the complex CEI and the short-lived reacting species.

Reviewer 3:

The reviewer detailed that the approach in this project is based on understanding that processes at the electrode/electrolyte interface, such as metal dissolution, oxygen evolution, and hydrofluoric acid (HF) attack, need to be investigated in situ, near electrode surface in order to unravel mechanistic details of these processes. Therefore, the approach here is to develop an electrochemistry-based characterization method that would enable characterization of the processes occurring at the electrode/electrolyte interface in situ. The reviewer said that the method is called SECM. This method could enable detection and analysis of the short-lived species generated at the electrode/electrolyte interface that could contribute to the battery performance degradation.

Reviewer 4:

The reviewer detailed that this project uses electrochemical microscopy to elucidate phenomena related to CEI, especially transition metal dissolution. The technique proposed provides unique insight and the plan of action is feasible. However, according to the reviewer, the PI should consider refocusing the effort toward materials with greater relevance to high energy batteries, moving completely away from Mn spinel to NiMn spinel or NMCs. Mn spinel is a very mature material where the existing barriers are rather low value.

Reviewer 5:

The reviewer said that the approach to the technical work is reasonable given the goals of understanding surface dissolution processes in lithium manganese oxide ($LiMn_2O_4$) The application of SECM and e-AFM is valuable in general; however, these techniques must be paired with extensive other materials characterization methods to improve scientific understanding as well as prove there is practical relevance to working on “model systems.” So far, the reviewer foresees challenges in connecting the results of these surface science techniques to produce a mechanistic level understanding, particularly as Mn dissolution is only one small part of the electrochemical process.

Reviewer 6:

The reviewer detailed that the project is part of the Frontier Science effort of VTO to understand and control CEI for high energy density/high voltage cathodes where little is known about the nature and dynamics of CEI that may or may not form at the interface. The reviewer said that scanning electrochemical microscopy (SECM) as a technique is fine for studying this aspect of electrochemical batteries, but studying Mn dissolution from $Li_2Mn_2O_4$ as a starting point does not seem to directly address the technical barriers. Yes, there are some disagreements about the valency of the dissolved Mn, but this issue has been studied as much as any cathode issue, and there is published evidence recently demonstrating Mn ion presence in the SEI at the anode. The reviewer remarked this topic appears to have been picked to test out the new SECM and see what it can do in the hands of the NREL staff. There are lots of publications using SECM as a technique—it is not a new technique at all—to elucidate fundamental electrochemistry. The reviewer encouraged the NREL team to be bold in their approach to this project and target some of the advanced SECM techniques that could be applied to the formation and dynamics of CEIs and not just settle for studying Mn dissolution—even as a first step it does not make much sense to start here.

Reviewer 7:

The reviewer commented that the PI realized that SECM will not gain new or useful information on the reactions near the surfaces due to limitation of tip size. It is also not clear whether combined SECM/AFM can do the job.

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 this is a new project, and the work and accomplishment are as planned.

Reviewer 2:

The reviewer remarked the project has recently started, and progress is appropriate given the timeframe.

Reviewer 3:

The reviewer remarked this is a newly started project and off to a good start with baseline thin film cathode synthesis and initial demonstration of the CEI degradation probing.

Reviewer 4:

The reviewer said that the slides provided through PeerNet were different from those provided in the poster. Based on the former, progress has been good and in line with proposed milestones, although Milestone 2 was difficult to evaluate as written. The reviewer said that based on the latter, the third milestone of FY 2019 is on track.

Reviewer 5:

The reviewer said that some progress has been made—thin-film model materials have been made a couple of different ways and initial SECM experiments have been conducted in the short time that the project has been going. The reviewer said that this pace of activities needs to be accelerated however if the project is to have a reasonable chance to reach its stated objectives in a meaningful way. $LiMn_2O_4$ is a very well-known material and the possibility of identifying a collaborator who can provide the material without NREL having to produce it in-house should be considered so that the technical accomplishments can be focused on SECM analysis of the complex and coupled electromechano chemistry occurring at CEIs at high voltages. The reviewer said that similarly, finding collaborators who can provide fluorinated electrolytes or other non-standard electrolyte (e.g., concentrated or otherwise heterogeneous electrolytes) would greatly increase the value of this SECM-based project.

Reviewer 6:

The reviewer pointed out that the project started in October 2018; this is the first project period. $LiMn_2O_4$ electrodes have been chosen as the first material to investigate degradation processes. The reviewer detailed activities. First, baseline $Li_xMn_2O_4$ material samples have been prepared using sputtering deposition and polymer assisted deposition for initial characterization of Mn dissolution and understanding of the mechanism of this process. Second, SECM is installed in NREL Electrochemistry Laboratory in the glovebox environment. Initial bench level quantification is demonstrated. Third, while not included in the slides, the poster has also shown study of the $LiNi_{0.5}Mn_{1.5}O_4$ electrodes and experiments to understand the nature of the species forming due to manganese dissolution. The reviewer noted because this approach is based on electrochemical measurements, which generally only detect electrons that are being involved in the processes occurring in electrochemical system, more specifically at the electrode/electrolyte interface in this project, it is necessary to combine the measurements via SECM method with other techniques such as chemical analysis. It is important to be able to decouple signal in SECM method to attribute it to different processes occurring at the electrode electrolyte interface. The reviewer said this can be only done by integrating SECM with other electrode diagnostics approaches, and encouraged the team to establish collaborations or develop such diagnostics in-house.

Reviewer 7:

The reviewer remarked this project was very recently started, so there are not extensive results yet available. Good progress has been made in generating model surfaces for study through the polymer assisted deposition process. However, these require substantial characterization beyond what has been shown (i.e., AFM and XRD) are not sufficient as one must also show the composition of the surface and distinguish the local crystalline facets that are outward facing). The reviewer suspected that the polycrystalline nature of these surface will make it difficult to distinguish the mechanistic origin of Mn dissolution. Furthermore, SECM does not have a resolution high enough to generate such a picture. The reviewer said that E-AFM is better, but again needs to be paired with other techniques that show surface states in addition to morphology (e.g., Raman spectroscopy). The reviewer remarked that along these lines, it will be critical to connect processes detected electrochemically to physical phenomena—notoriously difficult and will likely require the use of even more fundamental model systems (i.e., polished Mn surfaces with and without oxygen, non-Li+ containing electrolytes). The reviewer said that the team may think about including a modeling portion of work to support their experiments. As none of these issues have been tackled, it appears premature to think about moving to NMC cathodes in which the electrochemistry is even more complex.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that the team is interacting well and communication is appropriate.

Reviewer 2:

The reviewer said good synergy exists between the growth capability at New Mexico State University (NMSU) and the analytical skills at NREL.

Reviewer 3:

The reviewer remarked collaboration across partner teams appears good.

Reviewer 4:
The reviewer said that the collaboration within the team is fine—it is clear that all of the team members are engaged despite not all of them being at NREL, but this project is very high risk and there is a real need for outside collaborators to maximize the impact of the project. The reviewer referenced a prior comment, and said the team should consider focusing on the SECM advances and relying on external collaborators to provide model materials and solvents. The thin-film format has shown time and again to be a useful model for real-world electrode reactions—so there are lots of people worldwide who know how to make thin-film materials with stunning precision, including staff at NREL. The reviewer remarked that kind of additional collaboration would accelerate progress on the SECM work. Further, the CEI is a very complicated and complex interphase—and so much less is known than the corresponding SEI. Accordingly, said the reviewer, multi-modal characterization—that includes SECM—will be required to unravel and control the CEI structure, composition, and dynamics. Having only SECM data will provide a piece of the puzzle, but alone it will have very limited impact. The reviewer said that any opportunity to integrate these SECM results with other's results from other techniques (from within the VTO program or not) should be identified and pursued. The reviewer said publishing the SECM work as standalone results will delay its impact by many years—the best citation is one that does not have to be made because the parties involved are working closely together.

Reviewer 5:
The reviewer remarked that the multi-institutional team, while noted, would benefit from a relevant computational collaboration at the scale of interest.

Reviewer 6:
The reviewer pointed out that the current team consists of researchers at NREL and NMSU. It would strengthen this project if the roles of participants were better explained. The reviewer noted that as explained in the Technical Accomplishments and Progress section, collaboration with groups that can carry out, for example, chemical analysis, is necessary to decouple different processes at the electrode/electrolyte interface.

Reviewer 7:
The reviewer had no comment.

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 the project is well planned with the forthcoming tasks (e.g., SECM system re-configuration and stud Mn-dissolution as a first baseline study).

Reviewer 2:
The reviewer remarked the proposed future research will take advantage of the experimental methods being used for the program.

Reviewer 3:
The reviewer remarked that to enable imaging/topography characterization, NREL's microscopy group is purchasing a combined SECM/AFM to obtain high-resolution data on samples. The reviewer detailed that future work will include study of the Mn-containing cathodes with different electrolyte formulations and deconvolution of the overlapping processes. Processes, mechanisms, and approaches learned and established for $LiMn_2O_4$ and $LiNi_{0.5}Mn_{1.5}O_4$ cathodes will be applied to investigate NMC-family high performing cathodes.

Reviewer 4:
The reviewer remarked the project would notably benefit from an acceleration toward cathode materials with relevance to high-energy batteries, leaving the Mn spinel quickly aside. The PI should consider aligning closely with other thin film efforts in this DOE program to achieve such acceleration, where NMCs are the target. The reviewer remarked the plan of action did not present any decision points or alternative pathways.

Reviewer 5:
The reviewer said that future work is too focused on adding incremental understanding to the dissolution of Mn from $LiMn_2O_4$. While this topic can be briefly explored to discover the full capabilities of the SECM and SECM/AFM instruments, the goal should be to get to the more strategically important NMC-type materials and CEI formation under high voltage as quickly as possible.

Reviewer 6:
The reviewer remarked it is a high-risk project due to the limitation of SECM.

Reviewer 7:
The reviewer said that being that the project recently started, much work remains and there appear few concrete decision points or milestones, and transitioning to e-AFM is clearly useful as its resolution is superior to SECM. More importantly, however, the team must give further consideration to connecting local crystallinity and composition to electrochemistry in order to provide value. The reviewer remarked that moving to NMC systems is more relevant from an application perspective, but it is premature to consider this without first mastering the mechanistically simpler $LiMn_2O_4$ system, which has only a single dissolving element. The reviewer remarked that additional consideration should also be given to how the CEI (varying based on synthetic method as well as electrolyte composition, etc.) will influence the ability to conduct SECM and e-AFM experiments.

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

Reviewer 1:
The reviewer said that the research is relevant to the DOE efforts in developing Li-ion batteries with high energy density, and high power density. In particular, this project addresses an important issue of Mn dissolution during cycling of highly performing transition metal oxide cathode materials containing Mn, such as NMC. If successful, this project will have a high impact on understanding of the mechanisms of the processes, such as Mn dissolution, at the electrode electrolyte interface; which is particularly important for the high-performance commercially utilized NMC-family cathode materials. The reviewer remarked that understanding degradation mechanism will lead to developing strategies to create Li-ion battery cathodes with enhanced performance.

Reviewer 2:
The reviewer pointed out that understanding of interfaces is an important need for the program.

Reviewer 3:
The reviewer noted that fundamental understanding the reaction between electrolyte and active materials is critical to a better battery.

Reviewer 4:
The project is aligned with the goal to achieve high-stability cathodes for improved Li-ion battery performance and life.

Reviewer 5:
The reviewer remarked this project could address the need to understand cathode decomposition mechanistically, but the relevance will depend on the ability to measure dissolution and interface formation

phenomena and explain them independently. Moving to more NMC cathode systems would also be more relevant, when appropriate. Impacts may include better design of cathodes to promote safety and cycle life.

Reviewer 6:

The reviewer commented that in a broad sense, the project's final goal does support DOE objectives to enable high capacity, high power safe rechargeables for vehicle electrification. The reviewer said that the initial work on Mn dissolution is far less supportive, but the project will hopefully quickly progress to the strategically important electrodes and electrolytes that address the CEI issue effectively.

Reviewer 7:

The reviewer remarked this project targets new understanding of interfacial phenomena at CEIs. While focusing on materials with modest relevance to DOE goals, the knowledge could be extended to more relevant systems, especially if the objects of study were redefined much earlier than planned.

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 team has adequate access to the proposed resources.

Reviewer 2:

The reviewer said resources for this project are sufficient.

Reviewer 3:

The reviewer said resources are sufficient for the proposed program.

Reviewer 4:

The reviewer said yes, and commented the project has the resources to achieve the stated milestones, but management of the project will have to keep the project focused efficiently on the most strategically important work—otherwise the countless number of new opportunities that are less strategically important but sure to arise in a frontier science project will absolutely drown out this chance for success.

Reviewer 5:

The reviewer said the team has some adequate resources to carry out this research; however, some of the resources either still need to be purchased (SECM/AFM capability) or established (integration with chemical analysis). The latter are currently in progress.

Reviewer 6:

The reviewer had no comments.

Reviewer 7:

The reviewer had no comment.

Presentation Number: bat427
Presentation Title: In Operando Thermal Diagnostics of Electrochemical Cells
Principal Investigator: Ravi Prasher (Lawrence Berkeley National Laboratory)

Presenter
Ravi Prasher, Lawrence Berkeley National Laboratory

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

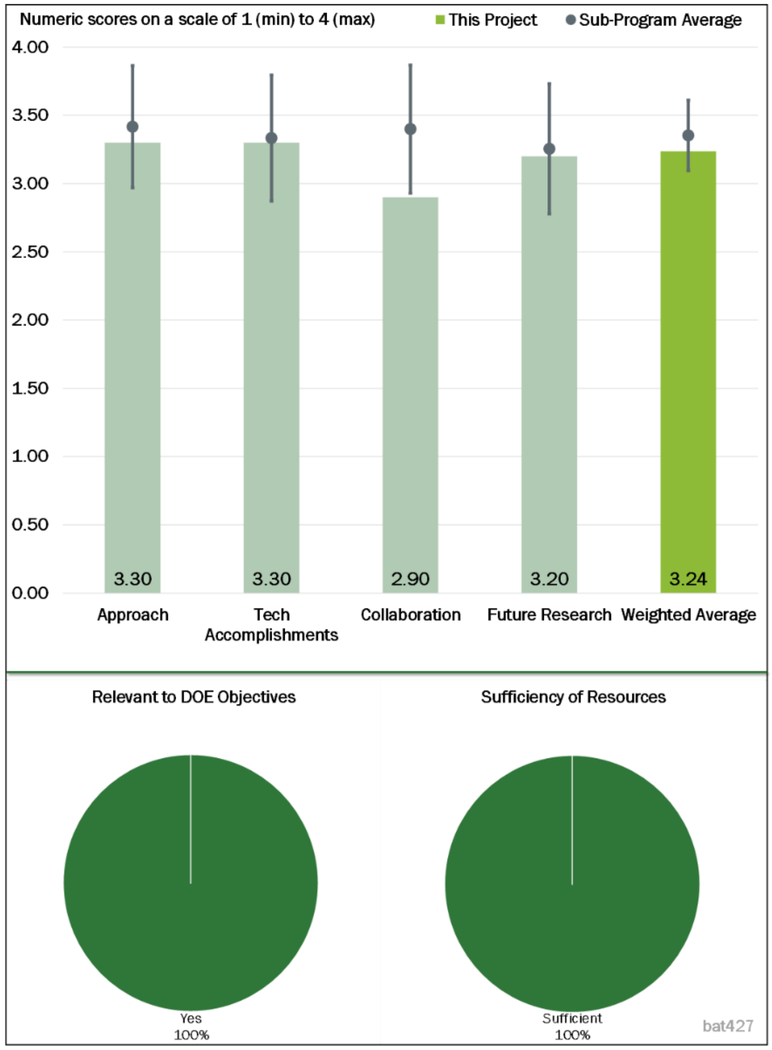

Figure 2-82 – Presentation Number: bat427 Presentation Title: In Operando Thermal Diagnostics of Electrochemical Cells Principal Investigator: Ravi Prasher (Lawrence Berkeley National Laboratory)

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 noted that the approach of using 3-omega method for thermal conductivity measurement for electrochemical cells is novel, though the same technique has been used for many other applications.

Reviewer 2:
The reviewer said that the program seems to be progressing well, and it is a relatively small effort.

Reviewer 3:
The reviewer commented the program is well designed to develop the operando measurement technique to measure the thermal transport properties within batteries, which properly addresses the technical barriers. The method uses the sensitivity of heating frequency to the layer/interface positions. However, according to the reviewer, there may be a risk to detect a fast-charging battery. Overall, the project is rationally designed. The program is well designed to develop the operando measurement technique to measure the thermal transport properties within in batteries, which properly addresses the technical barriers. The reviewer said that the method uses the sensitivity of heating frequency to the layer/interface positions. However, there may be a risk to detect a fast-charging battery. Overall, the project is rationally designed.

Reviewer 4:
The reviewer remarked the stated approach is to develop metrology to understand the source of the thermal bottleneck for fast-charge. The PI correctly points out that the need for high conduction as external cooling system alone will not save the team during fast-charge transients. That is good as far as it goes. The small thermal source/sensor is a nice idea. However, according to the reviewer, the planned work only identifies the source of thermal resistance in the cell (separator-electrode interface) without really understanding it. The

reviewer would like to see more investigation of that fundamental question as part of the experimental design, so that it can be mitigated.

Reviewer 5:

The reviewer remarked the work has shown the operando technique to measure thermal transport in a cell. The team's work shows that the highest thermal resistance is seen at the cathode/separator and anode separator interface. This work has also developed models to correlate their experimental results. This is interesting work and many challenging questions need to be answered to fully understand the thermal transport in Li-ion batteries. For example, the team claims that the thermal resistance is at the separator/electrode interface. However, this could still be a result of several factors. The reviewer said it would be interesting if the team performed studies to investigate different separators, electrolytes, and electrolyte additives, and separator coatings. This would help identify what is actually attributing to the increased thermal resistance. Additionally, according to the reviewer, it is unclear how the state of charge (SOC) or discharge changes the thermal transport. Locally on the surface of the anode and cathode could be higher thermal resistances due to the movement of Li and the interfacial resistances there.

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 progress seems appropriate to the budgeted amount.

Reviewer 2:

The reviewer said results presented appear to be highly promising.

Reviewer 3:

The reviewer remarked the key technical accomplishments of identifying the dominant factor in determining the thermal resistance of the battery and in operando measurement have been properly achieved according to the project progress. All milestones have been met so far. The reviewer commented that technical accomplishments made in the project are satisfactory.

Reviewer 4:

The reviewer remarked it appears that most of the time was spent developing the metrology and little has been done in providing serious insight in how to enable fast-charging. The PI appears to be meeting milestones. The reviewer pointed out that prior work has already shown that separator-cathode interface is the thermal bottleneck (see https://doi.org/10.1016/j.jpowsour.2015.09.028) so that is not necessarily new, though the in situ confirmation provided by this work is nice.

Reviewer 5:

The reviewer said the team has been able to show and model the thermal transport in a single layer pouch cell. This work is great and creating the model was an important accomplishment. There are several questions that are raised now to address what the team has found. The reviewer said that when talking to the presenter, it seems that these are challenges the team has acknowledged but is not necessarily set to explore. Namely, understanding what the exact mechanism is of the thermal resistance increase, specifically, is it the separator, electrolyte, or interface. Additionally, per the reviewer, when the team mapped the thermal transport it was unclear as to what SOC the results were taken. This could change depending on the SOC and should be investigated.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the small team appears to be highly collaborative and effective.

Reviewer 2:
The reviewer said that collaboration appears to be okay, and not much would be expected from such a small program.

Reviewer 3:
The reviewer said that the team has shown good work on developing the technique, but it is unclear how the team has used their collaborators to improve the work.

Reviewer 4:
The reviewer remarked the team needs to strengthen its collaboration in order to accomplish this project more efficiently.

Reviewer 5:
The reviewer said little or no evidence was given of collaborations outside (or even inside) 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 remarked that proposed research is well planned and on-track to meet objectives.

Reviewer 2:
The reviewer remarked the goal and steps for future research are quite specific.

Reviewer 3:
The reviewer said the proposed future research on measurement from both cathode and anode sides and detailed operando measurement is effectively planned and reasonable.

Reviewer 4:
The reviewer thought the planned future work was good, especially the "hoped" parts on how to understand and improve the thermal resistance, but would like to see more specifics on the physical origins of thermal performance. When the reviewer asked about this there were a couple ideas given but they were unclear. For instance, even just comparing thermal resistance to a few different cell compositions or chemistries might give insight when one compares those that are worse to those that are better. The reviewer said that because we are focusing on the electrode/separator interface, thin-electrode cells could be used to maximize sensitivity. Also, there could be some three-dimensional (3D) modeling analysis of how this dominating resistance affects transient heat profile in spirally wound 18650 cell. The reviewer asked are there any cell design approaches that could mitigate the problem if it cannot be solved at the interface level.

Reviewer 5:
The reviewer said proposed future work of operando 3ω measurements and more detailed measurements seems vague and needs to be focused more. The team claims that the interface is contributing to 65% of the batteries' thermal resistance and understands what components (i.e., electrolyte, separator, SOC, etc.) are needed to lay out a more fundamental experimental plan.

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

Reviewer 1:
The reviewer noted that the PI makes a good case that thermal limitations are highly relevant to fast-charge and need to be understood to be mitigated.

Reviewer 2:
The reviewer remarked that enabling fast-charge can increase adoption of EV technology.

Reviewer 3:
The reviewer pointed out that building and understanding operando thermal transport is important for diagnosing safe Li-ion batteries. The team has developed the tool and now need to perform more detailed work to show what is causing the large thermal resistances seen.

Reviewer 4:
The reviewer said that the project is very helpful to enable extremely fast-charging.

Reviewer 5:
The reviewer remarked the project well supports the DOE objectives, as the proposed project focuses on thermal diagnostics of 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 the team seems to have sufficient resources.

Reviewer 2:
The reviewer remarked resources are sufficient considering the scope of the program.

Reviewer 3:
The reviewer said the resources for the project are adequate to achieve the milestones timely.

Reviewer 4:
The reviewer remarked the team seems to have sufficient resources.

Reviewer 5:
The reviewer said the team seems to have adequate resources to perform the operando testing, and perhaps the team needs to have more electrochemists to help in identifying the anomalies they are seeing.

Reviewer 6:
The reviewer remarked the PI appears to have needed access to what is needed to complete the project as stated. Additional collaborations with cell-building people could help.

Presentation Number: bat431
Presentation Title: Investigation on Lithium Superoxide-Based Batteries
Principal Investigator: Khalil Amine (Argonne National Laboratory)

Presenter

Khalil Amine, Argonne National Laboratory

Reviewer Sample Size

A total of two reviewers evaluated this project.

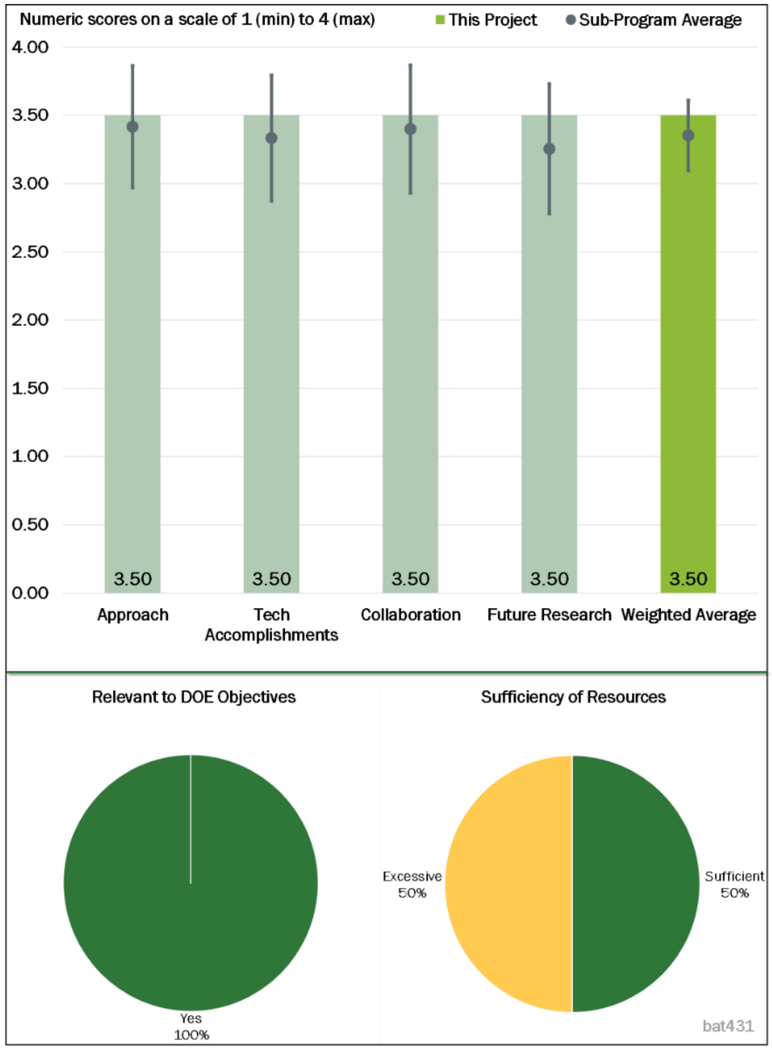

Figure 2-83 – Presentation Number: bat431 Presentation Title: Investigation on Lithium Superoxide-Based Batteries Principal Investigator: Khalil Amine (Argonne National Laboratory)

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 detailed that the PI and associates used both numerical calculation and analytical methods to investigate an electrochemical system of superoxide. Both numerical and experimental techniques are used to investigate the fundamental mechanism of conversion reaction, especially how to stabilize the superoxide. The reviewer noted that superoxide decomposition kinetics may be investigated.

Reviewer 2:

The reviewer said that the sodium (Na) work is interesting, but researchers need to remember that "long cycle life" is relative. While 118 cycles may be an accomplishment for lab tests, it is important to remember that the ultimate goal of battery research is to produce cells capable of 1,000's or 10,000's of cycles. The reviewer remarked early stage research in understanding battery technology is important, but should always be done with the ultimate product goal in mind.

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 two superoxide systems were investigated: sodium superoxide (NaO_2) and lithium superoxide (LiO_2). The mechanisms of the systems are investigated and elucidated. The reviewer remarked both NaO_2 and LiO_2 were partially stabilized. A cathode with cobalt(II, III) oxide (Co_3O_4) containing Li_2O was studied as a cathode material. The reviewer said that the accomplishment exceeded expectation.

Reviewer 2:

The reviewer said that Ir work was documented, but results and their implication on battery understanding and future design was not as clearly explained. The reviewer pointed out that two slides on the Ir work appeared in duplicate in the slide deck, perhaps that was in error and further explanation of the Ir results were intended to be added with explanation of continued battery research building on the results of that work.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer said that the PI has collaborated with researchers of both Argonne National Laboratory (ANL) and universities, and the collaboration is adequate and synergetic. The reviewer suggested including an industry collaborator.

Reviewer 2:

The reviewer remarked notes and publications indicate that the researchers collaborated with the partners on the project 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 the PI proposed to study electrolytes suitable for superoxide, continue the investigation of the conversion reactions of both NaO_2 and LiO_2, and expand the research to potassium superoxide (KO_2). The proposed future research is in-line with the project goal and well contemplated.

Reviewer 2:

The reviewer said that the proposed future work seems logical; however, the reviewer would encourage a targeted study of electrolytes in superoxide-based batteries, rather than systematic. Past research should be used to optimize future direction, and that path should be clearly articulated in review materials. The reviewer said that given the remaining project time, focused research on Na, versus Na and K systems, may optimize research results and understanding.

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

Reviewer 1:

The reviewer remarked the proposed project aims to understand the fundamental conversion mechanism of a novel kind of chemistry using alkali metal superoxide including NaO_2, KO_2 and LiO_2 as an active material in high-energy batteries. The research is relevant to the goal of DOE to develop a high energy system to support long distance driving per charge.

Reviewer 2:

The reviewer said yes, although a clear path to a final battery product should be articulated to help frame the context of research and a clear direction toward goals.

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

Reviewer 1:

The reviewer said that resources are supporting the completion of milestones in a timely fashion.

Reviewer 2:
The reviewer remarked that as a National Laboratory, ANL can provide more than adequate resources for the PI and team to conduct the proposed research.

Acronyms and Abbreviations

$/kWh	Dollars per kilowatt-hour
3-D	Three-dimensional
5M	Five molarity
µL/mg	Microliter per milligram
µm	Micron
AC	Alternating current
AFM	Atomic force microscopy
Ah	Amp-hours
Al	Aluminum
Al_2O_3	Aluminum oxide
ALD	Atomic layer deposition
ALS	Advanced Light Source
AMR	Annual Merit Review
ANL	Argonne National Laboratory
APS	Advanced Photon Source
ASI	Area specific impedance
BCDI	Bragg-coherent diffraction imaging
BCP	Block co-polymer
BEV	Battery electric vehicle
BMR	Battery Materials Research
BMS	Battery management system
BNL	Brookhaven National Laboratory
BOL	Beginning of life
C	Coulomb
CAE	Computer-aided engineering
CAEBAT	Computer-aided engineering of batteries
CAMP	Cell Analysis, Modeling, and Prototyping Facility

CC/CV	Constant current/constant voltage
CE	Coulombic efficiency
CEI	Cathode-electrolyte interphase
CF_3-EC	1-(trifluoromethyl)ethylene carbonate
CFN	Center for Functional Nanomaterials
cm	Centimeter
CMC	Carboxymethyl cellulose
CNT	Carbon nanotube
Co	Cobalt
CO_2	Carbon dioxide
$Co_2Ni/LiOH$	Cobalt and Nickel particles embedded in LiOH as a catalyst
Co-Ex	Co-extrusion
Cr	Chromium
CY	Calendar year
DEMS	Differential electrochemical mass spectroscopy
DFT	Density functional theory
DOD	Depth of discharge
DOE	U.S. Department of Energy
D_s	Diffusion coefficient
DSC	Differential scanning calorimetry
EB	Electron beam
EC	Ethylene carbonate
ED	Electron diffraction
EEI	Electrode-electrolyte interface
EELS	Electron energy loss spectroscopy
EERE	Energy Efficiency and Renewable Energy
EET	Electrical, electrochemical, and thermal
EIS	Electrochemical impedance spectroscopy

EMC	Ethyl methyl carbonate
EOL	End of life
E-S	Electrolyte-sulfur
EV	Electric vehicle
F	Fluorine
FEC	Fluoroethylene carbonate
FIB	Focused ion beam
FOM	Figure of Merit
FTIR	Fourier transform infrared
FY	Fiscal year
GC-MS	Gas chromatography mass spectroscopy
GM	General Motors
Gr	Graphite
GSIR	Gas-solid interface reaction
HCE	High-concentration electrolytes
HEV	Hybrid electric vehicle
HOH	Highly ordered hierarchical
HOMO	Highest occupied molecular orbit
HPPC	Hybrid pulse power characterization
HRTEM	High-resolution transmission electron microscopy
i_0	Exchange current
ICL	Irreversible capacity loss
ICP-MS	Inductively coupled plasma mass spectroscopy
IMRI	Irvine Materials Research Institute
INL	Idaho National Laboratory
IR	Infrared
JPL	Jet Propulsion Laboratory
kg	Kilogram

kJ/mol	Kilojoules per mole
L_2S	Lithium sulfide
LBNL	Lawrence Berkeley National Laboratory
LFO	Li_5FeO_4
LFP	Lithium-iron phosphate
Li	Lithium
Li_2CO_3	Lithium carbonate
Li_2O	Lithium oxide
Li_2S	Lithium sulfide
Li_3N	Lithium nitride
LiBOB	Lithium bis(oxalato)borate
$LiCoO_2$	Lithium cobalt oxide
LiF	Lithium fluoride
LiFSI	Lithium bis(fluorosulfonyl)imide
LiO_2	Lithium superoxide
LiOH	Lithium hydroxide
LiPAA	Lithium polyacrylate
LiPON	Lithium phosphorus oxynitride
$Li\text{-}SiO_2$	Lithium-silicon dioxide
LisTFSI	Lithium bis(trifluoromethanesylfonyl)imide
$Li_xP_yS_z$	Organo-lithium-phospho-sulfide
Li_xSi	Lithium silicon
Li_xS_y	Organo-lithium sulfide
LLTO	Lithium lanthanum titanate
LLZO	Lithium lanthanum zirconate
LMR	Lithium-manganese rich
LPS	Lithium phospho-sulfide
LRLO	Lithium-rich layered oxide

LRTM	Lithium-rich transition metal
LUMO	Lowest unoccupied molecular orbit
mAh	Milliamp-hour
mAh/cm^2	Milliamp-hour per square centimeter
mAh/g	Milliamp-hours per gram
MCA	Multicomponent alloy
MD	Molecular dynamics
Mg	Magnesium
mg	Milligram
mg_s/cm^2	mg_{sulfur}/cm^2
Mn	Manganese
MS	Mass spectroscopy
N/A	Not applicable
N:P	Negative-to-positive ratio
N_2	Nitrogen
NASA	National Aeronautics and Space Administration
Nb	Niobium
NCA	Nickel cobalt aluminum oxide
NDA	Non-disclosure agreement
NERSC	National Energy Research Scientific Computing Center
Ni	Nickel
NMC	Nickel manganese cobalt oxide
NMP	N-methyl-2-pyrrolidone
NMR	Nuclear magnetic resonance
NREL	National Renewable Energy Laboratory
O_2	Oxygen
OCP	Open-circuit potential
OCV	Open circuit voltage

OEM	Original equipment manufacturer
OEMS	Online electrochemical mass spectroscopy
ORNL	Oak Ridge National Laboratory
PAA	Polyacrylic acid
PEGDA	Polyethylene (glycol) diacrylate
PEO	Polyethylene oxide
PEO-PS	Polyethyleneoxide-polysulfide
PF_6	Hexafluorophosphate
PHEV	Plug-in hybrid electric vehicle
PHI	Physical Electronics Inc.
PI	Principal investigator
PNNL	Pacific Northwest National Laboratory
POSS	Polyhedral oligomeric SilSesquioxane
PPS	Porous polyethylenimine
PQILE	Polymer in “quasi-ionic liquid” electrolyte
PS	Polysulfide
PSU	Pennsylvania State University
PVDF	Polyvinylidene difluoride
Q	Quarter
R&D	Research and development
RIXS	Resonant inelastic X-ray scattering
s	Second
S	Siemen
S	Sulfur
Se	Selenium
SAW	Surface acoustic wave
SBR	Styrene butadiene rubber
SEI	Silicon electrolyte interface

SEI	Solid electrolyte interphase
SEISta	Silicon Electrolyte Interface Stabilization
SEM	Scanning electron microscope
SHP	Self-healing polymer
Si	Silicon
SIA	Structurally isomorphous alloy
SIMS	Secondary ion mass spectroscopy
SiO_x	Silicon oxides
Si-Sn	Silicon-tin
SLAC	Stanford Linear Accelerator Center
Sn	Tin
SNL	Sandia National Laboratories
SOC	State of charge
SOH	State of health
SPRDE	Stationary probe rotating disk electrode
SSE	Solid-state electrolyte
SSRL	Stanford Synchrotron Radiation Lightsource
STEM	Scanning Tunneling Electron Microscopy
S_xSe_y	Composition of Sulfur and Selenium in a composite
Ta	Tantalum
TBA	Tetrabutylammonium
TEM	Transmission electron microscopy
Ti	Titanium
TM	Transition metal
TNO	Titanium niobium oxide
TOF	Time of flight
U.S.	United States
UCB	University of California at Berkeley

UK	United Kingdom
UMEI	University of Michigan Energy Institute
USABC	U.S. Advanced Battery Consortium
UT	University of Tennessee
UV	Ultraviolet
V	Vanadium
V	Volt
VASP	Vienna Ab initio Simulation Package
VC	Vinylene carbonate
VTO	Vehicle Technologies Office
Wh/kg	Watt-hour per kilogram
WPI	Worchester Polytechnic Institute
wt. %	Weight percent
XANES	X-ray absorption near-edge structure
XAS	X-ray absorption spectroscopy
XCT	X-ray computed tomography
XFC	Extreme fast charging
XPS	X-ray photoelectron spectroscopy
XRD	X-ray diffraction
Zn	Zinc