2. Energy Storage Technologies

Energy storage technologies, especially batteries, are critical enabling technologies for the development of advanced, fuelefficient, light- and heavy-duty vehicles, which are critical components of the U.S. Department of Energy's (DOE's) Energy Strategic Goal: "to protect our national and economic security by promoting a diverse supply and delivery of reliable, affordable, and environmentally sound energy." The program's vision supports the development of durable and affordable advanced batteries covering the full range of vehicle applications, from start/stop to full-power hybrid electric, electric, and fuel cell vehicles. Much of this work will be applicable to energy storage for heavy hybrid vehicles as well. Energy storage research aims to overcome specific technical barriers identified by the automotive industry and the Vehicle Technologies Program. These include cost, performance, life, and abuse tolerance. These barriers are addressed collaboratively by DOE's technical research teams and battery manufacturers.

In August 2009, DOE announced the selection of 26 projects (totaling \$1.5 billion) for expanding U.S. manufacturing capacity for advanced batteries and advanced battery components. These American Reinvestment and Recovery Act (ARRA)-funded projects support establishing a significant domestic capacity for batteries that will, in turn, help commercialize advanced electric drive vehicles. Twenty of those ARRA projects focus on developing manufacturing capacity for advanced batteries and battery components (including the production of lithium-ion cells and polymers), production of polymer separators and other components, and battery recycling. The six remaining projects focus on the creation of new battery facilities, or the upgrading of existing facilities, to enable researchers to test batteries, improve battery safety, and increase the throughput of specialized thermal testing.

During this merit review, each reviewer was asked to answer a series of questions using multiple-choice responses (and with explanatory comments when requested), as well as using numeric scores (*on a scale of 1 to 4*). In the following pages, reviewer responses to each question for each project are summarized, the multiple choice and numeric score questions are presented in graph form, and the explanatory text responses are summarized for each question. The summary table below lists the average numeric score for each question and for each of the projects.

Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
† A High-Performance PHEV Battery Pack	Mohamed Alamgir (LG Chem, Michigan)	2-5	3.25	2.50	2.50	3.00	2.75
† USABC LEESS and PHEV Programs	Leslie Pinnell (A123Systems)	2-8	2.67	2.33	2.33	2.33	2.42
† JCS PHEV System Development-USABC	Avie Judes (Johnson Controls-Saft)	2-10	3.33	3.33	3.33	3.00	3.29
† Multifunctional, Inorganic- Filled Separators for Large Format, Li-ion Batteries	Richard Pekala (Entek)	2-12	4.00	3.75	3.75	3.00	3.72
Engineering of High Energy Cathode Materials	Khalil Amine (Argonne National Laboratory)	2-14	3.25	3.00	3.00	3.00	3.06
New High Energy Gradient Concentration Cathode Material	Khalil Amine (Argonne National Laboratory)	2-17	3.20	2.60	2.60	3.20	2.83
Development of High-Capacity Cathode Materials with Integrated Structures	Michael Thackeray (Argonne National Laboratory)	2-20	3.25	3.00	3.00	3.00	3.06
Developing A New High Capacity Anode With Long Cycle Life	Khalil Amine (Argonne National Laboratory)	2-22	2.00	2.25	2.25	2.25	2.19
High Voltage Electrolytes for Li- ion Batteries	Richard Jow (Army Research Laboratory)	2-25	3.25	3.00	3.00	3.25	3.09
Development of Advanced Electrolyte Additives	Zhengcheng Zhang (Argonne National Laboratory)	2-28	2.75	3.25	3.25	2.50	3.03

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Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
Electrolytes for Use in High Energy Lithium-Ion Batteries with Wide Operating Temperature Range	Marshall Smart (Jet Propulsion Laboratory)	2-31	4.00	3.75	3.75	3.25	3.75
Novel Phosphazene Compounds for Enhancing Electrolyte Stability and Safety of Lithium-ion Cells	Kevin Gering (Idaho National Laboratory)	2-34	2.67	3.00	3.00	2.67	2.88
Screening of Electrode Materials & Cell Chemistries and Streamlining Optimization of Electrodes	Wenquan Lu (Argonne National Laboratory)	2-36	2.60	2.80	2.80	2.80	2.75
Scale-up and Testing of Advanced Materials from the BATT Program	Vince Battaglia (Lawrence Berkeley National Laboratory)	2-39	2.80	3.40	3.40	3.40	3.25
Fabricate PHEV Cells for Testing & Diagnostics	Andrew Jansen (Argonne National Laboratory)	2-42	3.00	2.67	2.67	3.00	2.79
Electrochemistry Cell Model	Kevin Gallagher (Argonne National Laboratory)	2-44	3.00	2.75	2.75	2.25	2.75
Diagnostic Studies on Lithium Battery Cells and Cell Components	Dan Abraham (Argonne National Laboratory)	2-46	3.33	3.67	3.67	3.00	3.50
Electrochemistry Diagnostics of Baseline and New Materials	Robert Kostecki (Lawrence Berkeley National Laboratory)	2-48	4.00	3.33	3.33	3.33	3.50
Diagnostic Studies to Improve Abuse Tolerance and Life of Li- ion Batteries	Xiao-Qing Yang (Brookhaven National Laboratory)	2-50	3.33	3.00	3.00	3.33	3.13
Develop and Evaluate Materials and Additives that Enhance Thermal and Overcharge Abuse	Zonghai Chen (Argonne National Laboratory)	2-52	2.67	2.67	2.67	2.67	2.67
Evaluation of Abuse Tolerance Improvements	Chris Orendorff (Sandia National Laboratories)	2-54	3.67	3.67	3.67	3.33	3.63
Overcharge Protection for PHEV Batteries	Guoying Chen (Lawrence Berkeley National Laboratory)	2-56	3.33	3.00	3.00	3.33	3.13
† Inexpensive, Nonfluorinated (or Partially Fluorinated) Anions for Lithium Salts and Ionic Liquids for Lithium Battery Electrolytes	Wesley Henderson (North Carolina State University)	2-58	3.67	3.33	3.33	3.67	3.46
† Molecular Dynamics Simulation and AB Intio Studies of Electrolytes and Electrolyte/Electrode Interfaces	Dmitry Bedrov (University of Utah)	2-61	4.00	3.67	3.67	3.67	3.75
† Nanoscale Heterostructures and Thermoplastic Resin Binders: Novel Lithium-Ion Anodes	Prashant Kumta (University of Pittsburgh)	2-64	4.00	3.00	3.00	3.00	3.25
† Metal-Based, High-Capacity Lithium-Ion Anodes	Stanley Whittingham (Binghampton University-SUNY)	2-66	3.00	3.50	3.50	3.50	3.38
† Electrolytes - Advanced Electrolyte and Electrolyte Additives	Khalil Amine (Argonne National Laboratory)	2-68	3.67	3.00	3.00	3.00	3.17
† Development of Electrolytes for Lithium-ion Batteries	Brett Lucht (University of Rhode Island)	2-70	3.50	3.50	3.50	3.00	3.44
† Bifunctional Electrolytes for Lithium-ion Batteries	Daniel Scherson (Case Western Reserve University)	2-72	3.50	3.00	3.00	3.50	3.19
† Polymers For Advanced Lithium Batteries	Nitash Balsara (Lawrence Berkeley National Laboratory)	2-74	3.00	3.33	3.33	3.33	3.25

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Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
† Electrolytes - R&D for Advanced Lithium Batteries. Interfacial Behavior of Electrolytes	John Kerr (Lawrence Berkeley National Laboratory)	2-76	4.00	4.00	4.00	3.33	3.92
Diagnostic Testing and Analysis Toward Understanding Aging Mechanisms and Related Path Dependence	Kevin Gering (Idaho National Laboratory)	2-79	3.40	3.00	3.00	3.00	3.10
Overview and Progress of United States Advanced Battery Research (USABC) Activity	Kent Snyder (Ford Motor Company)	2-82	3.67	3.67	3.67	3.33	3.63
Progress of DOE Materials, Manufacturing Process R&D, and ARRA Battery Manufacturing Grants	Chris Johnson (National Energy Technology Laboratory)	2-84	3.00	3.00	3.00	3.00	3.00
† Electrolytes and Separators for High Voltage Li Ion Cells	Austen Angell (Arizona State University)	2-86	3.33	3.00	3.00	3.00	3.08
PHEV Battery Cost Assessment	Kevin Gallagher (Argonne National Laboratory)	2-88	3.67	3.00	3.00	3.33	3.21
High Voltage Electrolyte for Lithium Batteries	Zhengcheng Zhang (Argonne National Laboratory)	2-90	2.75	3.00	3.00	2.75	2.91
Spherical Carbon Anodes Fabricated by Autogenic Reactions	Michael Thackeray (Argonne National Laboratory)	2-92	3.00	2.75	2.75	2.50	2.78
Novel Composite Cathode Structures	Christopher Johnson (Argonne National Laboratory)	2-95	2.50	2.75	2.75	3.00	2.72
Overview of Computer-Aided Engineering of Batteries (CAEBAT) and Introduction to Multi-Scale, Multi-Dimensional (MSMD) Modeling of Lithium-Ion Batteries	Ahmad Pesaran (National Renewable Energy Laboratory)	2-97	4.00	3.67	3.67	3.33	3.71
Development of Computer- Aided Design Tools for Automotive Batteries	Steven Hartridge (CD- Adapco)	2-99	3.50	3.50	3.50	3.00	3.44
Development of Computer- Aided Design Tools for Automotive Batteries	Taeyoung Han (General Motors)	2-100	4.00	3.67	3.67	3.67	3.75
Development of Cell/Pack Level Models for Automotive Li-Ion Batteries with Experimental Validation	Christian Shaffer (EC- Power)	2-102	4.00	4.00	4.00	3.00	3.88
Open Architecture Structure for CAEBAT	Sreekanth Pannala (Oak Ridge National Laboratory)	2-105	3.67	3.00	3.00	3.33	3.21
Energy Storage Monitoring System and <i>in situ</i> Impedance Measurement Modeling	Jon Christophersen (Idaho National Laboratory)	2-107	3.67	3.00	3.00	3.00	3.17
Battery Ownership Modeling	Jeremy Neubauer (National Renewable Energy Laboratory)	2-109	2.33	2.67	2.67	2.33	2.54
Developmental and Applied Diagnostic Testing	Kevin Gering (Idaho National Laboratory)	2-111	3.67	3.33	3.33	3.67	3.46
† Electric-Vehicle Battery Development	Herman Lopez (Envia)	2-113	3.67	2.67	2.67	3.00	2.96
† EV Battery Development	Nick Karditsas (Cobasys)	2-115	3.00	2.67	2.67	3.00	2.79
† LEESS Battery Development	Kimberly McGrath (Maxwell)	2-118	3.00	3.33	3.33	3.00	3.21
† Novel High Performance Li-ion Cells	Keith Kepler (Farasis)	2-121	3.67	2.67	2.67	3.00	2.96

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Presentation Title	Principal Investigator and Organization	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
† 3-D Nanofilm Asymmetric Ultracapacitor	Fraser Seymour (Ionova)	2-123	3.00	3.33	3.33	2.67	3.17
† Implantation, Activation, Characterization and Prevention/Mitigation of Internal Short Circuits in Lithium-Ion Cells	Suresh Sriramulu (TIAX)	2-125	3.33	2.33	2.33	1.67	2.50
† Novel Anode Materials	Jack Vaughey (Argonne National Laboratory)	2-127	3.50	3.50	3.50	3.50	3.50
† Development of Si -based High Capacity Anodes	Ji-Guang (Jason) Zhang (Pacific Northwest National Laboratory)	2-129	2.50	3.00	3.00	2.50	2.81
† Atomic Layer Deposition for Stabilization of Amorphous Silicon Anodes	Anne Dillon (National Renewable Energy Laboratory)	2-131	4.00	4.00	4.00	4.00	4.00
† New Layered Nanolaminates for Use in Lithium Battery Anodes	Yury Gogotsi (Drexel University)	2-133	3.50	2.50	2.50	3.00	2.81
† Synthesis and Characterization of Polymer- Coated Layered SiOx-Graphene Nanocomposite Anodes	Donghai Wang (Pennsylvania State University)	2-135	3.50	2.50	2.50	3.50	2.88
† Wiring up Silicon Nanoparticles for High- Performance Lithium-Ion Battery Anodes	Yi Cui (Stanford University)	2-137	3.50	3.00	3.00	3.00	3.13
† Synthesis and Characterization of Silicon Clathrates for Anode Applications in Lithium-Ion Batteries	Kwai Chan (SwRI)	2-139	4.00	3.00	3.00	3.50	3.31
Addressing the Voltage Fade Issue with Lithium-Manganese- Rich Oxide Cathode Materials	Anthony Burrell (Argonne National Laboratory)	2-141	3.80	3.60	3.60	3.40	3.63
Development of Industrially Viable Battery Electrode Coatings	Robert Tenent (National Renewable Energy Laboratory)	2-144	3.00	3.00	3.00	3.00	3.00
Design of Safer High-Energy Density Materials for Lithium- Ion Cells	llias Belharouak (Argonne National Laboratory)	2-146	3.00	3.00	3.00	3.25	3.03
Overcoming Processing Cost Barriers of High-Performance Lithium-Ion Battery Electrodes	David Wood (Oak Ridge National Laboratory)	2-148	3.00	2.67	2.67	2.67	2.75
Roll-to-Roll Electrode Processing and Materials NDE for Advanced Lithium Secondary Batteries	Claus Daniel (Oak Ridge National Laboratory)	2-151	2.33	2.33	2.33	2.67	2.38
Post-test Cell Characterization Facility	Ira Bloom (Argonne National Laboratory)	2-153	3.50	3.50	3.50	3.25	3.47
Process Development and Scale up of Advanced Cathode Materials	Greg Krumdick (Argonne National Laboratory)	2-155	3.50	2.75	2.75	3.50	3.03
Process Development and Scale up of Advanced Electrolyte Materials	Greg Krumdick (Argonne National Laboratory)	2-157	3.25	2.25	2.25	3.00	2.59
Overall Average † denotes poster presentation			3.31	3.08	3.08	3.06	3.14

† denotes poster presentations

A High-Performance PHEV Battery Pack: Mohamed Alamgir (LG Chem, Michigan) – es002

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Only one of the four reviewers directly addressed this question, saying that the relevance to DOE goals and petroleum displacement is clear. There is a substantial need for higher capacity and energy for lowering the cost of the 40-mile system. Comments of the other reviewers were much more narrowly focused on the internal goals and barriers of this project. One reviewer cited that the goals of this work were to implement higher-energy materials for improved Li-ion batteries (greater range) and to lower costs, one of the main barriers to the acceptance of this technology. This work was focused on the battery pack design, thermal management issues and on devising a complete product. It would form framework for а commercialization of new advances in materials and design. The other two comments were similar. One noted that the battery pack design determined the effectiveness of the pack in meeting the demands of the application. The other asserted that both high-voltage cathodes at the cell level (to maximize the energy and thus reduce the cost) and cooling systems at the battery pack level (to optimize performance, lifetime and safety) were crucial for pack development.



Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

With the exception of the first comment (which termed the design excellent, incorporating attention to the essential details of the needs), reviewer comments, while generally positive, were tempered with suggestions for the modification of the work approach. One reviewer noted that the development of a cold-plate refrigeration system was quite important and was proceeding on schedule. The work with a high manganese (Mn) cathode system, however, was far from complete with two-thirds of the time gone. The approach of lowering the upper and lower cutoff voltages has improved the cycle life at the expense of severe attrition of capacity. The use of additives has not shown sufficient improvement in the cycle life. The reviewer suggested that the principal investigator (PI) contact vendors of cathode materials to determine if better materials were now available. Continued work with Samples A and B was unlikely to result in the successful conclusion of the work. The third reviewer observed that the specified approach was to characterize high-capacity, Mn-rich, layered-layered cathode materials (obtained from several sources) in terms of performance, durability (cycle life) and abuse tolerance. A second project goal was to optimize a refrigerant-to-air cooling system developed earlier in the United States Advanced Battery Consortium (USABC) program. It was unclear to the reviewer why these unrelated tasks were included in the same project rather than being separated into two different projects. Nonetheless, the reviewer deemed both highly relevant to the successful development of viable battery packs for electrified vehicles. The last reviewer noted

that LG Chemical has developed a proprietary separator material that can enhance safety for large cells that will be used for electric vehicle (EV) batteries and the like. LG Chemical was also one of the first major companies to scale up and be ready to provide real batteries for this business. This work focused on the pack design and on switching to an air-cooled system from one that required a more costly and complex refrigerant system. LG Chemical was sampling Mn cathodes from commercial suppliers. Such materials were likely to be scalable and more relevant to production in the near term. However, they may not necessarily represent the leading edge of this technology. The techniques being used were fine (gas sampling, impedance, Mn solubility measurements and cell testing).

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

In this section too, one of the four reviewers commented simply that the design had been implemented and battery packs performed as required, while others called attention to the pressure of a tight schedule for accomplishing final project goals and to other perceived shortcomings. One reviewer reiterated a concern from the previous section, saying that as noted in the approach section, the accomplishments to date were far from meeting cycle life/capacity goals and the problem of voltage fade had not yet been addressed. The latter was an important feature of the high-manganese material, especially when discharged to below 2.5 volts as revealed in this review. The PI should consult with Argonne National Laboratory (ANL) personnel as well as with vendors to upgrade the program or there was little chance of achieving the goals. The third reviewer noted that cathodes from two different vendors were evaluated. The limited data provided suggested that the discharge cut-off (low) voltage significantly impacted the cycle life (4.4 V to 2.0 V is much worse than 4.4 V versus 3.2 V). The reviewer found this interesting, but noted that no indication was provided of why it was the case. The upper charging voltage (4.1 V to 4.5 V) also dramatically impacted the cycle-life due to severe Mn dissolution and considerable gas evolution. The well-known need for an improved electrolyte was noted. A rapid increase in the cell resistance was also noted at low state-of-charge (SOC), which may limit the usable SOC for a battery pack, but again the reviewer found no mention in the presentation of why this occurs, and wondered if it was under study. The rate capability (at 1°C) also seemed to strongly limit the obtained capacity. Electrolyte additives were noted to improve the cycle life, but the improvements were quite limited, with the lifetime extended from about 80 to 160 cycles before rapid degradation. The capacity degradation profiles suggested that some form of degradation event was initiated and then propagated in each subsequent cycle, leading to a rapid decrease in capacity with each subsequent cycle. The reviewer asked what diagnostics were being performed on this degradation mechanism, and what studies were underway, such as those done by Daniel Abraham (of ANL), in which cells were disassembled, the electrodes washed and new cells prepared with the electrodes and fresh electrolytes to determine if the degradation was due to irreversible changes in the electrodes or instead due to changes in the electrolyte, loss of lithium, etc. It was unclear from the information provided what advances had been made in the cooling system. The last reviewer felt that the project team had done some nice design work and developed an air-cooled pack with good temperature control. The reviewer mentioned that the team had also explored the performance of new materials and identified some shortcomings (in rate) and the severe tradeoff in cycle life by going to too high a charge voltage to boost driving range per cycle. The project team has studied and done a good job of characterizing the vendor cathode materials, although the project did not appear to have made any significant improvements (this is consistent with plans). The reviewer called attention to the fact that this program was well positioned to take advantage of improvements made by other material suppliers. Costing information from this program on actual packs should also be valuable.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The pattern established in previous sections was continued in this one. One reviewer noted simply that the pack met the requirements of the customer and did not elaborate. The other three reviewers commented at considerably greater length, identifying perceived shortcomings in the extent and depth of collaboration in this project. One said that the program seemed to have utilized the national labs mainly for testing purposes. The evaluation of a new material with serious deficiencies, such as the high-manganese material, needed a broad-based collaboration with those studying the material deficiencies. A second reviewer found nothing in the review document that indicated that collaborations and coordination with other institutions were part of this project, except for the mention of partners including Idaho National Laboratory (INL), Sandia National Laboratories (SNL) and the National Renewable Energy Laboratory (NREL). What form of partnership had occurred this past year, however, was not evident. The "Future Work" notes that cells would be delivered to the national laboratories for testing, and external validation was

highly desirable. It was likely that most of the work was done in-house, although the cathode materials had been provided by two vendors, so perhaps some exchange of information had occurred to better understand the material properties. The fourth reviewer noted that this was a commercial company, so collaboration was typically never going to be as open as with an academic institution or national laboratory. Even recognizing this, however, the reviewer was struck by the poor communication of needs to LG Chemical by the USABC companies with regard to the need for the cooling work. It was unclear to the reviewer (and the reviewer believed, to LG Chemical) whether having to incorporate cooling into the actual pack was really essential at this stage of development. Greater clarity by DOE and USABC on what was really needed could help clarify the mission and focus efforts on the truly critical needs of this program. This was especially important, the reviewer felt, in view of the large amounts of time and money spent on engineering work for these large pack modules. This criticism, the reviewer pointed out, was aimed at DOE/USABC, not LG Chemical.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer noted that the project team had demonstrated the ability to successfully design and deliver battery packs with the required performance. Another reviewer felt that the emphasis on improving high-voltage cathodes through surface modification and electrolyte composition/additives was a reasonable means of deriving further improvements, but since no details were provided, could venture no further judgment. The testing of battery packs both in-house and at the national laboratories was welcome, as noted above. The third reviewer noted the plans to look at surface modifiers for the cathode and new electrolytes and/or electrolyte additives to improve cathode stability and considered them good, although striking a common theme. Obviously, the reviewer acknowledged, LG Chemical could not share details of such plans publicly. One of the reviewer's concerns regarding coatings was that this material already had rate issues and while the coatings would likely greatly improve cycle life, that the coatings may also aggravate the rate problems. Suggesting that emphasis be placed on ensuring such coatings are kept very thin, the reviewer said LG may wish to evaluate ALD-coated materials, and that LG and others also try to evaluate Envia Systems' cathode material if that was possible from a business confidentiality and commercial viewpoint. The last reviewer commented that no details had been provided regarding the additives or electrolyte compositions to be tested. Furthermore, the approach to surface modifications of the cathode material was not revealed. The reviewer then suggested that the PI should try to take advantage of work already done in the surface modification field by several DOE contractors and national laboratory workers.

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

Three of the four reviewers considered the project resources to be sufficient. One called the project well-planned and executed. The other found it difficult to estimate if the funding provided was appropriate, as the full range of activities was not specified and only limited results were described. LG Chemical, however, was cost-sharing the project, indicating a contribution of considerable resources. Given the company's standing in the lithium battery industry, it could be assumed that the provided funding was on target to achieve the DOE's goals. The fourth reviewer termed the resources excessive, noting that this was a substantial award, but at least LG had to match this (presumably with in-kind staffing). Pack design work was obviously a lot more expensive than cell design as at least prototype molding/tooling for many components was needed to provide actual samples. Thus, the funding level seemed not too bad, although basically product development work was being subsidized here that normally would be funded internally by such large corporations.

USABC LEESS and PHEV Programs: Leslie Pinnell (A123Systems) – es003

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

None of the three reviewers mentioned the overarching DOE goal of petroleum displacement, although one referred to DOE's goals without specifying which goals the reference was to. That comment was that the development of prismatic pouch cells with long cycle life, long calendar life, high energy density and reduced cost was crucial for achieving the DOE's goals. The second reviewer spoke to the internal project goals, saying that the overall performance goals seemed within reach for the hybrid-electric vehicle (HEV) battery, even though the plug-in hybrid-electric vehicle (PHEV) program did not meet the cost and volume goals. The lifetime issues were still somewhat cloudy, particularly at elevated temperatures. The third comment was similarly focused. The reviewer said the goal was to improve cells and packs with the lithium iron phosphate (LFP) and graphite chemistry per the relevant metrics.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? One reviewer cited an aspect of the work approach for



particular praise, finding it gratifying to see that the PI was paying some attention to thermal issues for the HEV battery, as the high pulse requirements, particularly for a small battery, were likely to raise the temperature substantially. It appeared there was no provision for cooling this battery - even through air cooling - which may be a real shortcoming in the approach. The cost goals would still be difficult to meet, as neither of the PHEV batteries met these goals in the previous program. The second reviewer expressed skepticism concerning the focus of the project, and doubted that the LFP would be a major player for automotive applications in the long term. Also, this reviewer claimed, information regarding the approach taken was completely absent. The third reviewer voiced a similar criticism, saying that the review document provided was not in the format specified by DOE. It was therefore difficult to determine what the approach used to address the technical barriers was. The reviewer noted that this was likely considered to be proprietary. A second program (LEESS) was now underway which aimed to optimize materials, electrodes, cell design and module design. Again, few details were provided.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

All reviewers cited a lack of adequate detail in the presentation to support an assessment of technical accomplishments, although the first reviewer also noted that project deliverables had been provided. The reviewer said that little in the way of details had been provided due to the information being considered proprietary. Evidently, for the PHEV10 goals, the cells performed well, except for the low-temperature cold crank performance and cost. For the PHEV40 goals, the system weight, volume and cost were noted

as problematic. It was unclear why the low-temperature cold crank performance for these cells met the DOE goals, but not for the PHEV10 cells. High-temperature (55°C) operation also was a challenge. The deliverables for the project had been met and the project had been completed. PHEV cells developed during this program had been commercialized. The second reviewer noted that the project was behind schedule. The HEV spending was behind plans due to a delay in cell building activities. However, no reason for the delay was given, nor was a plan presented to make it up. This gave concern about completing the contract on schedule. Very little information -was provided- regarding the materials selected, the cell design considerations or the cell builds, not to mention results to date on cell tests, so it was hard to comment on progress in these areas as well. The last reviewer said the gap analysis showed mostly green, with some red. This reviewer further opined there was not enough data to judge this more clearly.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

One reviewer noted that cells and packs from the PHEV program were being tested at the national laboratories. Cell modeling partners (University of Texas at Austin and Khon Kaen University) were noted for the development of 3D electrochemical and low-temperature kinetics models, suggesting that some collaboration has occurred or would occur. Although not explicitly mentioning collaboration or coordination, the second reviewer welcomed the addition of the thermal modeling efforts to the program. The company had said little about the effects of temperature, but the testing results at 55°C for the PHEV program emphasized the need for such an effort. The last reviewer felt that minimal collaboration was evident.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer voiced particular concerns with the cycle life and calendar studies due to the delays in the program. These studies required considerable time and there was no room for course correction. The cost picture was also a concern for this program, especially for the larger batteries to be made – 3.8 and 6 Amp-hours (Ah). Most HEV batteries were considerably smaller and it suggested that cycle life may not be sufficient for a normal HEV operation. The other two reviewers both cited a lack of sufficient information in the presentation on which to judge the proposed future work. One noted that the PHEV program was complete and that the HEV LEESS program was in progress, but no information was provided regarding future activities for the coming year except that it would focus on cell testing and module assembly. The last reviewer said simply that very little information was given, so this could not be clearly judged.

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

Two reviewers called project resources sufficient; one deemed them excessive. The first reviewer assumed that whatever was responsible for the delay was now rectified and that the resources were now adequate, but no statement regarding this was presented. The second noted that extensive funding had been provided, with half of the project funding cost-shared. It could be expected that A123 was well-equipped to conduct the work specified in the project. For the LEESS project, the actual funding spent seemed to be well below the projected expenses due to a delay in cell build activities. The reviewer who believed resources to be excessive expressed the belief that funding was more than enough for the goal.

JCS PHEV System Development-USABC: Avie Judes (Johnson Controls-Saft) – es005

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

One of the three commenting reviewers called the project relevant to all of the USABC and DOE goals, but did not mention petroleum displacement specifically. The second noted that the JCI project, now completed, focused on improving a lithium-ion battery system for a PHEV. The resulting battery system design would enable a PHEV to go 20 miles without using gasoline before switching to a charge-sustaining mode, when the car would again use gasoline for propulsion. The work led to a battery with better cell energy, power densities, and capacity retention during cycle life testing which, if installed in a new PHEV, would help to make these vehicles more attractive in the commercial market. The third reviewer said that the objectives were met in a timely fashion, resulting in a PHEV pack with excellent performance.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer approved the approach of using a proposed standard cell size (EUCAR/VDA) for the work



to assess the capabilities of the size and dimensions. Since the add-on program was just beginning and the previous project was completed, the reviewer continued, evaluation of- the approach was limited to consideration of proposed future work. The investigation of higher-capacity materials and higher charge voltages was a good one. However, the limitations of the discharge cut-off voltage should be kept in mind by the investigators. It was assumed that the general approach for the previous program would be continued. Also noting that the project was completed (in June 2011) and a follow-on project had just begun, the second reviewer felt that it was clear that the project succeeded. The one place in which it appeared to this reviewer to have fallen short of initially stated objectives was that lithium-ion systems were supposed to have been developed for both 20-mile and 40-mile all-electric range applications. However, in the end, it was only a 20-mile range system that was delivered, and a design study for a 40-mile range system. The reviewer was unsure of the original wording of the objectives, but wanted to note this possible discrepancy. Otherwise, the group had successfully delivered its battery system to the national laboratories for testing, which was underway. The last reviewer's comment was that the project team had demonstrated professional capability in creating the design and building of a battery pack that met the objectives.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

One reviewer called the improvements in the cell and system performance over the course of this study significant, citing a five percent increase in cell energy, a 28% increase in power density, and a 21% decrease in resistance over the course of four builds of

the system. The second noted the successful design of a battery pack for PHEV applications and the third simply noted that a follow-on program was just beginning.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

One reviewer said it was helpful to work directly with suppliers such as Entek on separator development to bring in a costeffective element to the cell. This was the only comment that implied a judgment of the quality of the collaboration in this project. The other two reviewers mainly noted the collaborating institutions. One said JCI was collaborating with ANL, NREL, SNL and Entek International and expressed the understanding that most of the national laboratory collaboration consisted of the tests these labs were carrying out now that the 20-mile PHEV system had been delivered. The second said that the project team had utilized facilities at ANL, SNL and NREL, along with the separator developer Entek.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer referred to comments provided under the topic of Approach to Performing the Work, in which the reviewer had expressed approval of using a proposed standard cell size. The second reviewer cited the follow-on project launched in April 2012 that would focus on the cells only. This was not elaborated on in the posters, the reviewer noted, but rather shared by the presenters. The last reviewer also cited the just-commenced follow-on program, for which little detail was available.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? All three reviewers believed resources to be sufficient. One said the funds appeared to have matched the needs of the project. Another said the project was well planned by a professional organization.

Multifunctional, Inorganic-Filled Separators for Large Format, Li-ion Batteries: Richard Pekala (Entek) – es008

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Two of the four reviewers endorsed the project's support of DOE's petroleum displacement goal. One said Entek's development of an advanced separator design that would increase abuse tolerance, ruggedness and reliability while reducing cost would support the continued introduction of plug-in electric vehicles to U.S. roads, which would indeed support the DOE objective of petroleum displacement. Yes, said another, it supported the overall DOE petroleum displacement. The project moved battery technology closer to realworld situation. Nail penetration tests performed on cylindrical cells were very encouraging. The third reviewer, while not mentioning petroleum displacement explicitly, said that the objective of a low-cost separator that had excellent performance and safety was very compatible with goals. The last comment was that the reliability and life of batteries with robust separator technology for the electrified vehicle had been addressed during the poster presentation.

Question 2: What is your assessment of the approach to performing the work? To what degree



are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

In the view of one reviewer, this was a very novel project with a good chance of success. The approach to limit silica inclusion in an ultra-high molecular weight (UHMW) polyethylene separator was valid on a cost basis and the observed properties compared to other inclusions tried. The second reviewer noted that the abuse testing, which was so critical for these batteries, was showing nice progress. The overcharge test, oven ramp, short circuit and nail penetration tests were very encouraging. At some point the authors should give additional details about cost, about how this separator compared with standards ones. It seemed that the goal was \$1 per square meter. The remaining two comments were largely descriptive of the approach, without offering explicit assessments of its appropriateness. One reviewer said Entek was focused on making variations of its novel, inorganic-filled separator design that would be highly porous but would operate safely. After it makes its test separators and puts them into production runs of 18650 cells, it characterizes certain properties of these and sends the separators to the national laboratories for abuse testing to check their durability. The fourth reviewer observed that by employing different inorganic fillers in their separator, Entek has tried to improve life, safety and cost of lithium-ion batteries. The inorganic (ceramic) fillers help improve electrolyte adsorption, provide better mechanical integrity against high temperatures, and reduce the overall cost of the separator (depending on the choice of the ceramic fillers).

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

There has been important progress, said one reviewer. The improved cycle life, lowered self-discharge and higher rate capabilities were important milestones. It could be of great interest, this reviewer said, to know if those variables translated also when tested on prismatic cells. The second reviewer noted that the silica-filled separators do offer some improvement in performance over the control separators to which they are compared, but in other respects, the performance has not changed. Thus far, the new separators did not shut down and would not prevent cell over-pressure on overcharge, nor would they prevent thermal runaway. But they did increase the margins before failure. It was reported that cell cycle life was improved in some cases with use of this separator. The project had accomplished interim goals and was on track to continue, in the opinion of a third reviewer. The fourth reviewer observed that full cell tests had shown better life and performance of the cells. However, the ceramic filler separator did not offer dramatic improvement in terms of safety compared to Entek's current state-of-the-art separator.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewers gave this project generally high marks in this category. One reviewer called the collaboration outstanding, as all the major U.S. battery manufacturers were being supplied material and structural experiments were carried out as appropriate by nonbattery producer collaborators. Another cited good collaboration with universities, national laboratories and large cell makers for the full evaluation of the separator developed under this program. The third reviewer agreed, saying that the group had shown good collaboration. It was not easy to get industrial partners, but strong effort in that direction was important, in particular with battery companies. The fourth observed that Entek listed several partners who helped in some of the testing and measurements after Entek manufactures its separators. The bulk of the collaboration appeared to come from Mobile Power Solutions and SNL, both of whom were conducting abuse testing of the batteries containing the novel separators. These results were key to gauging the success of the new separator design.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Noting that different precursors and treatment methods would be further evaluated, one reviewer predicted that the evaluation of ceramic filler separators with a large format cells would provide useful information on this separator technology. Two reviewers offered suggestions for future research. One expressed interest in seeing some prismatic cell work done with wound electrodes to see if the separators could stand up to the small radius of curvature of the inner windings of this type of cell. Also, stacked cells with separator folds should be evaluated (e.g. Z-fold or wrapped units). Another noted that the authors mentioned pilot production in their presentation and wondered if they foresaw potential surprises if the process had to be scaled up. Cost issues, this reviewer said, should be mentioned with additional detail. Noting that a lot of results were presented with cylindrical cells, this reviewer also believed, with the presenter, that future results on prismatic cells may end up being very important. The last reviewer observed that the proposed future research continued along the same lines of trying new materials and then testing the cell performance and abuse testing. Entek will play with the parameters of its manufacturing process and then follow this with measurements and testing.

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

The four reviewers were unanimous in terming project resources sufficient. Two offered supplementary comments. One noted that the funding given to this project was comparable to the funding for a similar project developing inorganic separators for large-format lithium-ion batteries that Entek completed during 2010-2011. The other felt that with the resources that the project had received so far, the authors had shown good progress and a variety of testing and results. If the project scaled up the process, additional resources would be needed.

Engineering of High Energy Cathode Materials: Khalil Amine (ANL) – es015

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Three of four reviewers considered this project to be highly relevant to DOE's petroleum displacement goal. One said development of reliable, high-performance positive electrode materials was a critical element in the national effort to reduce petroleum consumption (provided the electricity comes from non-petroleum sources). The ANL materials for lithium-ion battery (LIB) cathodes were considered to be the current state of the art. This project, said the second reviewer, was very relevant, because it strongly addressed one of the top five technological barriers to reducing petroleum dependence, effectively targeting one of the key materials that need to be optimized for commercialization: high-energy, layered cathode materials. This project had correctly identified the key issues for this material, and the approach was excellent for finding solutions. The aluminum fluoride (AlF_{3}) coating was a step into a promising direction. The third reviewer agreed and said that the project was very relevant to the overall DOE objective of petroleum displacement. High-energy composite cathode materials were badly needed so that goal can be achieved. The last reviewer called it imperative for the success of the



program to have good high-energy cathode materials, but did not directly address petroleum displacement.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Reviewer comments on the work approach were generally positive. One reviewer said that the group was doing a good job in focusing on technical barriers. The cracking of particles produced through carbonate precipitation was a good example. In the future, it could be of interest if the project team offered additional details on that issue. The authors have shown great flexibility, the reviewer went on, and quickly moved towards the hydroxide precipitation process. In the view of the second reviewer, the project approaches were fairly well-organized in material synthesis/variation, scale-up and testing. The material characterization and scale-up partners looked very strong. However, the material had some issues concerning voltage loss and cycle life. The reviewer asked who was providing the fundamental understanding of the electrochemical properties. The third reviewer termed the AIF₃ nanoparticle surface decoration a step into a promising direction. Optimization of lithiation, transition metal ratios, crushability, and precursor route were all the right controls to address. The reviewer remarked that coordination of large-scale material production with a major cathode material vendor would be nice, and perhaps that was already happening. The fourth reviewer urged that the cost also be included as a factor. There was no point, the reviewer said, in pursuing cathode materials with high-cost raw materials.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewers offered some positive comments on the project's progress and technical accomplishments achieved to date, but overall, seemed to have more questions than opinions. One reviewer noted that both the voltage drop and cycle-life have been improved, but that both needed further improvement. The investigator believed that an electrolyte additive could solve the fade (i.e., manage Mn dissolution and plating on graphite), and that this may be corrected. The analysis and testing were very thorough, and very impressive. The second reviewer commented at considerable length, noting first that steady progress had been made in variation of synthetic processing and characterization, but felt that the effort lacked some fundamental understanding. For example, according to the formula as written, the first charging capacity could not exceed 200 mAh/g. However, the first charge injection/activation was about 300 mAh/g. The reviewer asked what was being oxidized at the 4.6 V plateau. X-ray absorption spectroscopy (XAS) data from Brookhaven National Laboratory (BNL) did not show any transition metal oxidation in that region. The reviewer continued to ask if oxygen was evolving from the material; if there were any gas detection plans; what the consequence of AlF_3 coating at two weight percent (2 wt%) was; and what the capacity trade-off in a given volume was. The scanning electron microscope (SEM) images showed rather thick coatings due to the relatively low density of the coating material. In the full cell test, the cell was losing about 33% capacity even with AlF₃ coating at 300 cycles, which fell far short of the PHEV target. The reviewer questioned what the degradation mechanism, dissolution of TM or particle cracking was. Moderately elevated temperature test hardly constituted an abuse tolerance test. The reviewer went on to question if there had been any examination of material degradation at 4.6 V for a prolonged time. The third reviewer noted that the authors were trying different approaches to address the difficult issues the researchers encountered as the project moved forward. Coating with AlF₃ was one of them. The stability issues were difficult to study and to solve. The high-energy powders were very important and badly needed in the industry. The reviewer suggested that at some point, the authors should mention the cost issue and some of the barriers that the project may encounter as it is scaled up. This reviewer asked if it would be easier to scale up a carbonate precipitation process compared with the hydroxide precipitation. At some point the authors should mention the minimal tap density the project can tolerate for these powders in practical applications. It seemed that tap density was an important variable when working with these powders. The final reviewer's comment was brief, observing that it would have been appropriate to compare dry nano-AlF₃ addition to other, more conventional procedures for coating with AIF₃ and decide whether this method was better, worse or the same.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Two reviewers commented positively on project collaboration. One said the project team had shown good interaction with other institutions, and added that it was not easy to find industrial partners. The second noted that the project included a good combination of national laboratories and industry. The third comment was that the project appeared to need some help on fundamental understanding from electrochemists. There were enough material scientists in the team. The fourth reviewer was unable to understand how the collaboration worked, namely, what contribution was made by the collaborators. The reviewer acknowledged that the collaboration may be good, but was unable to determine that.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Voltage fade seemed to be the critical issue, one reviewer observed. This was a difficult project because there was a lot of basic research and development activity mixed with a strong effort toward practical applications, scale-up work and the important issue of cost. At some point the authors should treat the last item in more detail. The second reviewer said simply: Good. The third, said that although the material appeared to be a very good candidate, it was not yet fully validated. Both the coating materials and the coating thickness must be optimized. The reviewer asked why the earlier carbon coating approach was abandoned. Also, this reviewer indicated that a plan to understand the degradation mechanism was needed. Overall, the reviewer suggested, DOE effort in this area (not just this project) may need a standardized protocol for material evaluation, including the abuse test.

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

Three of the four reviewers who commented thought the resources were sufficient; one termed them excessive. Two of the former three reviewers said, respectively, that this seemed reasonable – perhaps a little low, and that resources were probably sufficient. That could change if a promising solution was found for the voltage fade issue. If that happened, additional resources would be required to scale up. The reviewer who deemed the resources excessive noted that the ANL resources and those of the collaborators were enormous and mused that the project had the most resources in the world.

New High Energy Gradient Concentration Cathode Material: Khalil Amine (ANL) – es016

Reviewer Sample Size

This project was reviewed by five reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Most of the project reviewers provided similar comments regarding the project's relevance. One reviewer commented that new battery material development was good for petroleum displacement and that the ANL positive electrode materials were aligned with this effort. Another reviewer described the project as very relevant to the DOE objectives of petroleum displacement as the project concentrates its efforts on the cathode-one of the most important areas of lithium batteries-and on a novel powder for that cathode. This was reiterated by two other reviewers including one who explained that cathode materials (i.e., electrodes) with high capacity were one of the most promising approaches to reducing the overall cost of battery packs. The same reviewer noted that such materials must have high rate capability, durability (high stability) and safety (abuse tolerance) and that the gradient materials appeared to meet these demanding criteria. The other reviewer reinforced that development of high nickel (Ni) containing safe cathode materials was critical for the success of the plug-in electric vehicles/electric vehicles (PHEV/EV). The reviewer explained that the current



battery chemistry was very conservative and only a low level blending of Ni-containing cathodes was utilized. A different reviewer acknowledged that this project was a well-known concept, but that work needed to be done in this promising area.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Most reviewers provided similar comments on the project's approach to performing the work. One reviewer commented that this was an extremely creative approach to cathode modification to achieve the combination of properties (high energy density, high tap density, high rate capability, longer cycle life and improved safety) sought. This was partially reiterated by another reviewer who agreed that the approach was very innovative and appeared to have very good potential for high-volume manufacturing. Another individual acknowledged the researchers' strong effort to overcome barriers. In particular, the reviewer noted that the authors knew the problems that the project was facing, and that those problems were not easy. The reviewer claimed that it seemed that the most pressing one was to improve the stability of these powders to be able to scale up the process and cautioned that the scale-up process may provide some surprises; the amount of powder that may be out of spec should be kept to a minimum. Another reviewer asked the length of time that was required for the synthesis or how the project compared to the production of commercial cathode materials. The reviewer went on to question if it was reasonable to expect that this process could be commercialized at a reasonable production cost, which was also referenced by another reviewer. That reviewer suggested that the PI may want to consider the material manufacturing aspects of this approach such as cost and practicality. One of the reviewers

also mentioned that much of this work was and is being done by Dr. Sun in Korea and suggested that efforts should be made to describe how this work was different. A different reviewer pointed out that at this stage of the development, it might be necessary to not only focus on the optimization of the composition, but also to demonstrate the effect of the possible variability in the full gradient materials on the cell performance and safety and to define process parameters that must be controlled to reduce variability. Another reviewer pointed out that the approach of gradient shelling may improve the material stability by alleviating mechanical stress built in the particles/crystal lattice. On the other hand, one reviewer noted that the approach may not solve the issue of transition metal dissolution.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Most of the reviewers provided similar comments regarding the project's technical accomplishments and progress. One reviewer said that the project clearly demonstrated the benefits achieved using the gradient approach to cathode synthesis including a better cycle life, lower impedance growth and improved safety (due to lower heat generation). The reviewer particularly referenced that the cells performed well, even at 55°C. A reviewer indicated that the results obtained were very good for this time period and pointed out that the full cell cycling at high temperature was very impressive. Another reviewer commented that the technical accomplishments were numerous, and pointed out the high tap density powder reported for the core-shell with concentration gradient A (CSCG A) material was one of them and very interesting. The reviewer cautioned that one important challenge was to be able to scale up that process. The reviewer also added that the dynamic stress test reported for the core and full gradient material was very impressive. The same reviewer commented that the batch process implemented for the full gradient material seemed to be an important innovation; however, the reviewer expressed eagerness to learn additional details about the process (i.e., additional details related to the tap density of these powders). The reviewer commented that it was surprising to see the high tab density values observed for the gradient precursor obtained via CSTR. Another reviewer reiterated that the team had achieved amazing feats as demonstrated in the gradual atomic composition changes and the improvement in the cycle life. However, the reviewer also had some questions. One question was whether the presenters had any comments regarding the SEM images also showing material density gradient. The reviewer added that the presentation needed an explanation of cobalt role in the structure since its composition also changed from the core value. Another point mentioned by the reviewer was that the transition electron microscope (TEM) and electron diffraction (ED) data showed clearly different structures, but that TEM and ED were extreme local probes. Thus the reviewer questioned how much such a structure represented the overall material and opined that SEM micrographs covering a larger area could be more convincing. The same reviewer also remarked that the x-ray diffraction (XRD) pattern for the full gradient material was hard to understand. The reviewer noted that the shell lattice parameter was expected to be slightly different from that of the core and that diffraction peaks may be convolved and show some broadening. The reviewer questioned why the peaks were sharp and singlets. Other questions posed by the reviewer included what the charge-discharge rate for the full-cell tests were, if the PIs had projected energy density in the full cell configuration, and how it fit with DOE targets. Another reviewer observed that the researchers had addressed recommendations provided during previous reviews and had pursued a more advanced approach and shifted their focus from core-shell to full gradient materials.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments regarding project collaboration and coordination with other institutions varied. One reviewer felt that the team seemed to be very strong and pointed out that it was nice to see industrial partners involved in the project. In contrast, other reviewers criticized that the project had only a few collaborators, mainly foreign, and that more U.S.-based collaborations were desired. Another reviewer referenced that Hanyang University and ECPRO were noted as partners for the project, but that there was no information given with regard to what their role in the project was. The reviewer stated that no other mention of collaborations was made beyond the use of the ANL cathode scale-up facilities. The reviewer questioned if the materials had been shared with others for more extensive characterization. The reviewer cited as an example that sharing the material with the thermal safety team at SNL (i.e., Chris Orendorff - ES036) may be fruitful. A different reviewer also asserted that the PI may want to hear opinions on the practicality of the synthesis method from experienced material manufacturer.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments on the proposed future research were mostly positive. One reviewer summarized that the suggested work, including cathode synthesis with different surface concentrations and different gradient concentration slopes, tuning the thickness of the gradient and the Manganese (Mn)-rich shell, calendar and cycle life testing, safety testing and scale-up of the synthesis process were all well-aligned with the project goals. This was reiterated by another reviewer who indicated this was more critical since the approach generated promising results. Another reviewer indicated that the team seemed to be focused on the important issues of optimization of the hydroxide process, coatings, and voltage drop. A different reviewer recommended that a sample be coated with AlF₃ for comparison to other work being performed by ANL, even though more very good electrochemical performance was expected from the proposed work. Another reviewer suggested that in order to convince the industry to use this innovative technology it was important to compare performance/safety data versus industry baselines. For example, the reviewer questioned how LiMn₂O₄/NCA blend would compare to the full gradient composition having the same average composition as the current cathode mix composition and noted that the industry wants to see that simply coating or doping will not give the same results as the ANL technology. A different reviewer also suggested that to further address the density of these materials it might be important to evaluate the hydroxide versus carbonate route not only for the transition metal precursor but for the solid state lithiation reaction as well. One reviewer asked if once the material was prepared in larger amounts, it would be shared with other laboratories for testing. A reviewer also asked to have tests with fully configured cells and numbers on energy density.

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

All five reviewers felt that sufficient financial resources were available for the project. Two reviewers indicated that the project funding and resources available appeared or seemed to be sufficient for the work. However, one reviewer noted that if the authors came up with important developments that may overcome some barriers, that those may need additional funds. The reviewer noted that scale-up, for example, could be one of them.

Development of High-Capacity Cathode Materials with Integrated Structures: Michael Thackeray (ANL) – es019

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Three out of four reviewers provided similar comments on the project's relevance. One reviewer indicated that the development of reliable high performance positive electrode materials was a critical element in the national effort of reducing petroleum consumption if the electricity came from a non-petroleum source. The same reviewer noted that the ANL Li-excess material and its family were considered as the current state-of-the-art for lithium-ion battery (LIB) applications. Another reviewer pointed out that this project was addressing one of the key technology barriers for improving cell capacity, reducing cost, and reducing dependence on petroleum: improving high-energy layered cathode materials to make them commercially viable. Similarly, another reviewer commented that yes, the project objective was very much in line with petroleum displacement and that high capacity cathode materials played a critical role in this objective. The fourth reviewer indicated that the voltage fade issue needed to be resolved for these materials.

Question 2: What is your assessment of the



approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Yes (100%)

Most of the reviewers had similar comments regarding the project's approach to performing the work. One reviewer in particular commended that the project had a sound and methodical approach. Another reviewer mentioned that the synthetic efforts were first class; very interesting ideas designed to confront a very challenging problem such as the voltage fade phenomena. These comments were reiterated by another reviewer who commented that the ANL materials were known to be superior to others in the capacity. The reviewer mentioned that according to the PI's presentation, rate capability decays had been observed and suggested that a tactic to moderate the decay, particularly when the material was coated with AlF₃ may be needed. The reviewer also pointed out that fundamental understanding the degradation mechanism with charge-discharge cycles may accelerate the optimization effort in addition to the approaches such as coating or doping. A different reviewer suggested that looking at optimizing the composition with respect to adjusting the spinel content may be a fruitful direction. The reviewer however, expressed concern that it may be too constrained in terms of optimizing the ratios of the metals and the degree of oxidation of the initial material.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments on the project's technical accomplishments and progress varied. One reviewer noted that the project exhibited good progress. Another reviewer pointed out that the voltage fade issue was difficult but that the team was strong. A different reviewer

mentioned the loss of (ex-team member) Dr. Kang may impact the pace and hoped that the gap has been or would be filled by an equally capable investigator. A reviewer commented that it was excellent to examine area-normalized impedance and hoped that others to do the same in the impedance studies. A different reviewer pointed out that for the material formula as written, it was not possible to explain the first charge capacity of 250~300 milliamp hours per gram (mAh/g) but that despite such unknowns, the ANL layered material and its variation with spinel were superior positive electrode candidates for advanced LIBs. The same reviewer questioned if there was a significant oxygen deficiency that introduced Mn(III) in the pristine material or if oxygen was coming off at 4.6 volts. One of the reviewers indicated that it seemed that a lot of basic research was taking place now. At some point, the reviewer suggested that the authors should start mentioning some practical issues such as scale up procedures and cost. In addition, the reviewer recommended that the tap density measured on these powders be mentioned in future presentations as those values could give a hint on what to expect in terms of capacity on real battery electrodes. Another question posed by a reviewer was if there were any tactics to moderate the rate capability loss in the case of AlF₃ coatings or taking approaches of trade-offs among stability-capacity-rate capability. Another reviewer questioned if it would be helpful to add an electrochemist in fundamental understanding on the voltage loss mechanism. Other questions posed included whether or not the voltage loss related to transition metal-rich spinel phase accumulation and/or gradual Li-ion site changes from octahedral to tetrahedral. Also, one reviewer felt that the description of the results was a little ambiguous and unclear.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Two of the reviewers provided positive comments on the project's collaboration and coordination with other institutions noting that the collaboration team was well organized with external characterization resources and collaborations with other institutions seemed to be strong. One reviewer suggested that at some point, if the voltage fade issue gets partially resolved, that the authors should try a stronger interaction with industrial partners—the reviewer understands that those partners are not easy to find. One reviewer asked if it would be better to add a nascent electrochemist. Another reviewer reported not being able tell clearly how the collaborators contributed to the project.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer comments on the proposed future research varied. One reviewer commented that the future proposal was nicely focused on the issue. Another reviewer reiterated that the future direction was good, but was worried that continuing to work on composition optimization at the same time as exhaustively evaluating two leading compositions may be difficult. A different reviewer noted that there was a strong emphasis in understanding the main barriers related to these powders. The reviewer noted that at some point, as more progress was made on the mechanism involved on the voltage fade phenomena, additional efforts into the more applied field could be of great interest. One of the reviewers suggested that the project should also add Mg, and coat with AlF₃ to compare with similar ongoing ANL projects.

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

Three out of four reviewers felt that the project had sufficient financial resources available for the project. One reviewer felt that the project had insufficient financial resources. One reviewer thought that the ANL resources to develop advanced Li-ion materials are perhaps the best in the world. Another reviewer indicated that the resources appeared to be sufficient; however, warned that if important new developments were disclosed, that the authors may need additional resources to scale up or to test the powders in larger format batteries. The same reviewer remarked that this was a very important high energy cathode powder.

Developing A New High Capacity Anode With Long Cycle Life: Khalil Amine (Argonne National Laboratory) – es020

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewers expressed similar comments regarding the project's relevance. One reviewer indicated that large format batteries were required for the electrification of transportation and is one of the ways to reduce petroleum. Another reviewer mentioned that developing new anodes and understanding the details of its role in vehicle battery activity was important for optimized design and for real-world evaluation. A different reviewer summarized that the concept was to develop a new high capacity anode that would eventually lead to higher energy density batteries. The reviewer specified that tin and silicon were the most likely new anode materials to significantly improve battery energy density (run time) and that this work was mostly focused on tin.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project welldesigned, feasible, and integrated with other efforts? Comments on the project's approach to performing the work were mixed among reviewers. One reviewer acknowledged that the project's focus on silicon (Si) and



tin (Sn) was good, but that of course everyone else was doing this as well. Another reviewer commented that the results were promising, i.e., the capacity retention and cyclability of anodes made using ball-milled mixtures of few elements such as Sn, antimony (Sb), Si, carbon (C), and oxygen (O). The reviewer also suggested that as the materials preparation approach was somewhat fixed, the project looked at two of its aspects to improve the overall materials discovery approach further: develop a combinatorial approach to accelerate the understanding; and develop a rational basis for some of the targeted alloys through a number of means. A different reviewer mentioned that the PI had chosen carbon and oxides (MO)-Sn_xCo_yC₇ (MO=SiO, SiO₂), SnO₂, MoO₃, GeO₂) anode materials and tested them for possible application as battery anodes. The reviewer noted that the presenters claimed that Sn_xCo_yC_z alloys would provide a capacity of 400-500 mAh/g for hundreds of cycles and MO anodes could provide more than 1,000 mAh/g with poor cyclability. The reviewer added that the project approach, the formation of $Sn_xCo_yC_z$ and MO composite that could lead to the increase in the capacity, reduce the amount of cobalt in the material and improve the cyclability since $Sn_xCo_yC_z$ could play a role of buffer against the MO volume expansion had to be justified. The reviewer felt that the presentation results did not seem to show either high capacity or long cycle life time. Another reviewer indicated that the project basically seemed to be using a more concentrated (lower carbon content) variation of the Sony Sn/Co/C anode used in the Nexelion product characterized by Dr. Whittingham in 2006 as it essentially used the same Sn/Co approach. The reviewer added that while using more Sn/Co would indeed boost the energy of the system, the approach in the reviewer's view was flawed on two grounds. The reviewer pointed out that the cost of the cobalt in such an anode was far too high for the electric vehicle market to

absorb. As such, the reviewer opined that the approach was commercially a non-starter. Moreover, the reviewer asserted that the PIs did not explain just what the role of the cobalt was, presumably a stabilization effort. The reviewer reported that the presenters did talk about reducing the cobalt amount, but that this should have been a focus from the beginning, not when the project was about 70% complete. The reviewer reinforced that one of the goals was having a low-cost synthesis method, but that this would be pretty futile when using an expensive metal such as cobalt.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments on the project's technical accomplishments and progress varied. One reviewer noted that the project's technical accomplishments indicated reasonable results. Another reviewer reiterated that the data showed progress (i.e., developing alloys for high energy density anode). Another reviewer commented that the presenters were able to demonstrate good cycle life and that the possibility of having a Sn and Si alloy composition was potentially valuable, but only if the researchers could avoid the Co that goes along with the tin. The reviewer noted that capacities were decent, especially in view of the much better tap density of these anodes over carbon; however, the presenters did not provide or add any insight as to the role that Co played and/or how the same results could be achieved with less expensive elements. Another main concern of one of the reviewers was regarding the reproducibility of the materials proposed (i.e., as the materials were obtained in a manner that was probably not very reproducible, e.g., ball milling of mixtures of compounds). The reviewer asserted that this was because people may not be able to produce similar types of alloys (also not sure of the final state of alloys) even if people started with similar compositions of feed materials. Therefore, the reviewer suggested looking at alternate methods of obtaining alloys of such compounds (beyond ball milling) and/or running several trials to prove that this was something that is highly reproducible in terms of both electrochemical behavior (including voltage profile) and the alloys obtained. Additional comments were provided by another reviewer who indicated that certain specific comments were not addressed: the PI should clarify whether it was an alloy or a composite; the presenters needed to thoroughly characterize their system; having Co₃₀ in Sn₃₀Co₃₀C₄₀ system was not cost-effective; ultra-high energy ball milling machine (UHEM) did not seem to be cost-effective as well; the researchers needed to address the cost-effectiveness since the project's major goal was to develop a low-cost anode; the full cell test showed low specific capacity; and the researchers needed to explain how nanomaterials could decrease the solid electrolyte interphase (SEI) resistance and lead to higher specific capacities at high charge/discharge rates.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewers had mixed comments on the project's collaboration and coordination with other institutions. One reviewer remarked that the collaboration and coordination seemed to be fine. Another reviewer pointed out that it would be good to specify the nature of the work or what components of research were performed by the collaborators. Another reviewer commented that this project or work could easily benefit from interactions or collaborations with academic institutions. The reviewer suggested the following: develop interaction with strong materials research teams at an academic institution to develop a fundamental understanding of processing and final alloy produced. A different reviewer had different opinions and commented not seeing much evidence of significant collaboration, and acknowledged viewing collaboration as a means to an end (results) not an end in itself. The reviewer added not being sure that the project really warranted a lot of collaboration.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments on the project's proposed future research varied. One reviewer recommended that in addition to what was proposed in the presenter's original plan, the above suggestions (i.e., working with an academic partner for process-property relationship and/or developing some sort of rational understanding of the behavior) should be implemented. The reviewer noted that the project proposed to understand the causes of the first cycle charge discharge irreversibility and tried to reduce it, but that the project should also have to address how to improve the specific capacity. A different reviewer considered additional work on materials containing such high levels of Co worthy of intellectual curiosity only, and found it hard to support additional work in this area. The reviewer commented that this work needed to be redirected to look at commercially viable anodes, and in fact that this should

have been done much earlier in the program. The reviewer added that continuance of this project should occur if the project aggressively refocused on non-Co anodes.

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

Mixed comments were received regarding the adequacy of financial resources available for the project. Two of the reviewers felt that sufficient financial resources were available while the other two reviewers felt that financial resources were excessive. One comment made on the project's financial resources was that this work, from the reviewer's view, has not been very worthwhile and it was opined that funding should focus on work on anodes with little or no Co content.

High Voltage Electrolytes for Li-ion Batteries: Richard Jow (Army Research Laboratory) – es024

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Most of the reviewers provided similar comments on the project's relevance. One reviewer indicated that electrolytes capable of withstanding higher voltage environments are key to enabling the use of high voltage cathode materials for improved energy density. Likewise, the reviewer remarked that high voltage electrolyte should allow extension of battery life given electrolyte decomposition at voltage is a contributing mechanism of cycle life failure. Another reviewer pointed out that the investigation of high voltage electrolytes was very important for development of high voltage cathode in Li-ion battery technologies for increase in their energy density to enable compact, light, and cheaper electrified vehicles. This was somewhat reiterated by other reviewers. One reviewer indicated that higher performance (voltage and or capacity) are essential for future battery systems. The reviewer noted that present electrolytes lacked stability for higher voltage, higher performance systems. Another reviewer similarly remarked that stable electrolytes that could handle all the voltages that the electrode fabricators could come up with are clearly desirable. The reviewer



added that whether 5V should be a target was not clear as illustrated by the lack of reliable electrode supply and that it was not clear that 5V electrolytes were sensible. One of the reviewers also observed the project's need to identify additives as well as understand pathways and mechanisms.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Comments on the project's approach to performing had mixed reviews. One reviewer expressed that there was a good balance between the computational and experimental studies to better understand interfacial chemistry between a high-voltage cathode and electrolyte. Another reviewer remarked that the project involved the abilities of several people with excellent ability to identify new high energy materials, and further noted the double intercalation of each electrode. Other reviewers expressed similar sentiments in additional comments. Among those reviewers, one indicated that ultimately the section on additives for improvement of electrolytes in high voltage environments was interesting, but failed to cogently discuss mechanistic outcomes for the results. Another person stated that modeling of the solvent oxidation process seemed like it could be quite useful, however it was somewhat difficult to follow the logic train and conclusion in the presentation. A different reviewer felt that a huge amount of work had been done and a sensible balance of experiment and theory established. The reviewer pointed out that clearly the project was trying to do too much for the resources allocated and it should narrow down the areas of work. The same reviewer also pointed out that the anode theory work seemed to be out of place and that obviously more collaboration was required to leverage this work. A different reviewer questioned the inclusion of high-voltage cathode as a key element of the program and suggested that it might be better to take SOA high-voltage cathode from within the DOE/Army research infrastructure and just use best available. The reviewer noted that if the goal was to develop a high-voltage electrolyte, it might be best to just focus on that.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Mixed reviews were received regarding the project's technical accomplishments and progress. One reviewer discussed in detail that the project delivered the main reason for the decomposition of electrolyte solvent at high voltage and showed the effect of electrolyte additives on the battery life through this work. The reviewer noted that the information on the main degradation mechanisms in Li-ion battery technologies could be used for the development of robust electrolytes for better life and performance of cells and also was very useful to develop a semi-empirical battery model which gave a more accurate indication of battery life. The reviewer also suggested that verifying the reaction pathways and electrolyte degradation mechanism through this project could provide very useful information for the development of the next generation of lithium-ion battery technologies. Another reviewer indicated that computational efforts have identified a path to obtain better material performance. One reviewer in particular pointed out that the the additives HFIP significantly enhanced cycle life and Sldo strengthened SEI. A different reviewer remarked that the project identified a new material high energy intercalation phosphate cathode with improved performance capability and an additive that further improved performance. The reviewer added that the research stabilized LiCoO₄. One of the reviewers suggested using LiCoPO₄ as high voltage cathode material doped with Ferial to compare the stability results. In addition, one of the reviewers acknowledged seeing positive empirical results of the electrode additive on cycling performance but not getting the mechanistic tie-in. The reviewer questioned if it was due to the electrolyte stabilization, the anode stabilization or the cathode stabilization. The reviewer also commented that the mechanistic interpretation of stabilization could be stronger. A reviewer stated that it was a very productive project generating a lot of good data and theory, but noted that it was trying to do too much. Another reviewer agreed that the concept of a double intercalation cell is interesting but did not understand how the researchers got there, or more importantly, whether this was being well- understood. The reviewer suggested a significant review of previous work in this area and evaluation in order to suggest it as a viable direction.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewer comments on the project's collaboration and coordination with other institutions varied. One reviewer felt that the project had good coordination and collaboration with national laboratories, universities, and large battery makers for fundamental research and evaluation of new materials with large cells. Another reviewer felt that the project accomplished the goals with help from an excellent group of collaborators: ANL, University of Texas, University of Utah, University of Maryland, and Saft. This was reiterated by another reviewer who indicated that the collaboration options seemed adequate. One reviewer expressed that collaborations needed to be expanded greatly and beyond ANL, particularly for the theoretical underpinning.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer comments regarding the project's proposed future research varied. One reviewer felt that the investigation of reactions occurring at both positive and negative electrodes' interface would provide very useful information for the further development of lithium-ion battery technologies. Particularly, the reviewer noted that *in situ* characterization of SEI layer would give key information for the enhancement of battery life and performance. Another reviewer indicated that the project would continue with suggestions for successful implementation of new technology. A different reviewer had no major comments and hoped that future work would uncover reasons behind improved cathode stability with additives. A fourth reviewer felt that the future plans involved more of the same approach as before, which was not good. The reviewer added that the project should develop more collaborative work with a wider variety of partners or significantly narrow the scope and objectives.

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

Comments regarding financial resources varied. Three out of four reviewers felt that the financial resources were sufficient for the project. One reviewer indicated that the financial resources were insufficient. One reviewer indicated that the project had sufficient

resources and used them effectively. However, another reviewer felt that the financial resources for the project were not nearly enough to do everything. The reviewer added that this project needed to leverage other resources or should be much increased in funding.

Development of Advanced Electrolyte Additives: Zhengcheng Zhang (Argonne National Laboratory) – es025

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments for this section were mixed. One reviewer considered the answer to be a qualified yes. This reviewer felt that the goal of improving various performance parameters outlined in the discussion was of course relevant to the overall goal of the DOE. This questioned, however, whether additive reviewer development was the path that would provide the best outcome in the search for improved electrolytes. Another panelist remarked that discovery and application of additives that could improve the cycle and calendar life of the Li-ion batteries without having to make extensive changes to the present technology would be very valuable and help launch their use in the transportation arena where the lifetime issue was a major barrier. This panelist observed that the work involved trying to develop some simple rules combined with more fundamental considerations to develop methods of additive selection and screening that, if successful, would help the technology. The next observer wrote that electrolyte additives largely affected the life and performance of lithium-ion batteries. This observer recommended that, to enhance the life and performance



of lithium ion batteries, investigation of electrolyte solvents and additives needed to be carried out, since that would finally affect the cost of battery system. The final reviewer stated that the project objective was to develop an efficient, inexpensive functional electrolyte additive technology to address the barriers existing in the current Li-ion battery system, such as poor cycle life, calendar life and battery abuse tolerance. This reviewer suggested establishing structure-property relationship and calculations.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Reactions to this question were mixed. One reviewer thought that the approach was fine, stating that the candidate generation and screening characteristics were laid out well. This reviewer reported that two different paths (enablement and improvement) were described in the presentation. Another panelist related that electrolyte manufacturers usually made DOE (Design of Experiment) tables and evaluated new electrolyte components (solvent, salt, and additive) by running various life and performance tests with many samples cells containing new electrolyte chemistries. This panelist felt that electrochemical analysis, physical analysis, and theoretical approaches for better understanding of each electrolyte component's effect needed to be done, but suggested that making sample cells and evaluation of various electrolyte components was more practical and gave direct information on the effect of the electrolyte composition/chemistry changes. This panelist concluded that a lack of experiments for characterization (i.e. low temperature performance) of the proposed chemistry was evident. The next observer found that the approach was appropriate for a technology-based project. This observer reported that there was an attempt to combine fundamental theoretical considerations with

more empirical rules to guide the selection and application. This observer thought that the idea of screening a variety of related compounds to develop structure-function relationships was valuable and should be further pursued. That being said, the observer qualified that this approach was from classical physical organic chemistry which was a field that this reviewer knew personally and had examined some of the reduction reactions of these compounds. The observer further found no mention of the presenter consulting the very extensive literature developed back in the 60's and 70's, which would inform the selection. Similarly, this observer felt that the mechanism speculation was just that in the absence of proper product analysis and identification, much of which would be helped by reading the classical literature. The observer finally concluded that the project needed to build upon previous research and not try to reinvent the wheel. The final reviewer explained that work was directed at developing a new additive for the SEI layer formation. This reviewer also observed using the degree of unsaturation and heterocyclic compounds used for screening. The same reviewer also made note of the following: identifying four new compounds for further work; ANL-SEI-1 additive for SEI; and the synthesis of new additives.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments for this section were generally positive. One reviewer thought that the approach was well-thought out, logical and rigorous. This reviewer observed a good use of available tools to help build the data. This reviewer's only concern in the conclusions was that the additive benefit was displayed within an electrolyte which had no additives. The reviewer concluded by questioning if it was possible that already existing additive technology could provide the same (or higher) benefit. Another person found that it was hard to figure out tradeoffs with the proposed chemistry and again its effect on the battery life and performance needed to be validated without running the full spectrum of performance evaluation, even though new electrolyte additives showed an improvement in capacity retention. This person concluded that the AC impedance results indicated that the proposed chemistries may not improve the power capability of the cells. The next panelist reported the project had identified and produced additives effective in improving cell performance. The final observer stated that much work had been completed and much useful data had been generated. However, this observer found that the lack of cohesive theory to guide the work was impeding its usefulness, and that better controls were in order. The observer listed oxalato salts as an example as all the salts provided some reductive activity at about 1.6-2.0V, which EC did on its own. The observer explained that the commonality for this would be CO_2 reduction, and that controls using CO_2 , formate3, oxalate etc. would answer some of these questions. This observer concluded that the results were still very empirical and may be erroneous.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reactions to this question were mixed. One panelist found no major causes for concern, citing good use of various analytical tools that all seemed to be focused on the same question. Another panel member commented that there was considerable collaboration, but that some collaborators such as URI were not even listed. The next observer expected more collaboration with cell makers for a full evaluation of new chemistries. The final person reported that the project had engaged ANL DFT capability as well as the University of Utah, ARL, Conoco Philips, and Saft to help on particular segments of the work.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments for this section were mostly negative. One reviewer found the proposed future research to be more of the same, expanding into cathodes. This reviewer considered this not to be a good idea until a better understanding was gained. The reviewer suggested that perhaps this was a project where stronger links to BATT projects would be in order to gain a deeper understanding. Another panelist agreed that more of the same was proposed, and that a better baseline for success should be established first. The next observer felt that the researchers needed to make a decent DOE table for a more practical evaluation of new chemistries. The final panel member reported that the researchers would continue the development of new materials using quantum calculations and compound preparation for evaluations of new materials for overcharge protection and cathode additive materials, and that research would extend to overcharge protection and cathode additive.

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

Three reviewers found resources to be sufficient, and one rated them insufficient. A reviewer felt that a lot of work had been accomplished with small amounts of resources, and that resources actually may be insufficient if better understanding was desired. Another reviewer agreed that if anything the project could use more resources.

Electrolytes for Use in High Energy Lithium-Ion Batteries with Wide Operating Temperature Range: Marshall Smart (JPL) – es026

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments for this section were positive. One reviewer found this project provided an extremely effective testing capability for the evaluation of all kinds of electrolytes, modifications and additives in a proven cell system with reliable reproducibility. This reviewer felt that it was an essential component of electrolyte development necessary to expedite introduction of new and better electrolytes into the technology. Another panel member noted that for successful electrification of vehicles. batteries should be operated without compromising performance and life. This panel member explained that this work addressed practical issues most of lithium ion battery technologies faced such as poor performance and life at both high and low temperatures by employing novel electrolyte solvent blend and salt. The next panelist pointed out that cold temperature performance could get ignored in the discussion of Liion for motive power, but that it did matter and research that addressed this issue and provided some understanding of the options to mitigate was relevant.



The final observer reported that the project identified stable electrolyte systems for a 5V Li-ion cell at high and low temperatures and defined life-limiting mechanisms needed for advanced systems.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Reactions to this question were positive. One reviewer had no issues with the project, and called it well-done, comprehensive, and logical. This reviewer thought that it was probably the most comprehensive and well-presented talk of the session. Another reviewer remarked that the approach clearly defined the scope of work and characterized electrolytes through a range of electrochemical analyses. This reviewer found the researchers had finally evaluated the proposed electrolyte with both small- and large-scale lithium-ion batteries with different chemistries. The next panelist remarked that the project had a proven, reliable test system that allowed for evaluation of electrolyte changes in a reproducible fashion. In this panelist's opinion, the right experiments were done both in terms of cycle and calendar life combined with rate variation and impedance data. The panelist concluded that the data was very usable for the modeling community and hence provided an invaluable output. The final reviewer characterized the research as having defined 5V system requirements; having optimized carbonate solvent blends, fluorinated esters, and fluorinated carbonates solvents of low viscosity, low melting ester-based co-solvents coupled with novel, alternative lithium based salts (with USC, LBNL); and having ionic conductivity and cyclic voltammetry measurements: performance characteristics in 300-400 mAh

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three electrode cells MCMB/LiNi_{0.8}Co_{0.2}O₂, MCMB/LiNi_{0.8}Co_{0.2}AlO₂, Graphite/LiNi(1/3)Co(1/3)Mn(1/3)O₂, and Graphite/LLC-LiNiCoMnO₂; use of high specific energy; Electrochemical Impedance Spectroscopy (EIS) Measurements as function of temperature, high temperature storage, and cycle life; DC Tafel and linear (micro) polarization measurements on electrodes; exsitu analysis of harvested electrodes (URI and Hunter College); performance characteristics in coin cells Evaluation of electrolytes in conjunction with high voltage cathodes; and performance evaluation in prototype cells Yardney, A123, Saft, and/or Quallion Cells (0.300 mAh to 7 Ah size prototype cells).

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewers left positive comments in this section. One panelist thought that an outstanding amount of data was generated. This panelist felt that the fundamental understanding was clearly not present in the project, but that it provided large amounts of data in a reliable fashion that could be used by the entire community to understand the most variable of the components: the electrolyte. Another reviewer commented that the proposed electrolyte compositions seemed to work well with LFP chemistry but showed room to be improved for NCM chemistry. The last panel member thought that cold temperature performance enhancement looked promising as compared to baseline electrolyte performance on nickel based cathodes. This panel member noted that iron phosphate results were also interesting and useful to have an understanding of. This panel member concluded that this was a pretty good talk filling an interesting niche, and appreciated the rigor and quantity of the data presented.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reactions to this question were generally positive. One reviewer reported that the researcher had partnered with certain wellknown groups in battery electrolyte area. This reviewer saw a close collaboration with large battery manufacturers, other national labs and universities for a thorough evaluation of proposed electrolyte chemistries. Another reviewer found no issues with the project. This reviewer stated that a wide variety of chemistry from several different sources, both commercial and laboratory, were evaluated. The next panelist said that the project was clearly developing a client base so that developers of new electrolytes could have their new materials rapidly and accurately tested. This panelist thought that this was a major plus for both the DOE and the NASA programs. The next person listed collaborators as Dr. Lucht from the University of Rhode Island; Khalil Amine (ANL); and team members from NREL, SNL, and the Hunter College. The final reviewer reported that the researchers had performed electrochemical characterization of Graphite/Toda 9100 LiNiCoMnO₂ three-electrode experimental cells with methyl butyratebased electrolytes; evaluated a number of methyl butyrate-based electrolytes in Conoco A12 Graphite/Toda HE5050LiNiCoMnO₂ three-electrode cells (Argonne materials); and evaluated Methyl propionate and Triphenyl phosphate additives. This reviewer further reported that the MB-based formulations containing LiBOB delivered the best rate capability at low temperatures, and that the use of lithium oxalate as an additive gave the highest reversible capacity and lower irreversible losses. This reviewer further reported that at lower temperatures and higher rates, the advantages of utilizing the high voltage system diminished when compared to a standard NCA material. This reviewer further reported that LLC-NMC electrodes (received from Argonne) displayed much slower lithium de-intercalation kinetics.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments for this section were mixed. One reviewer believed that the search for alternative salts could have a higher priority in the overall scheme of electrolyte research, and hoped that this area of future work was followed diligently. Another observer felt that future research would be more of the same, which was all that could be expected for the current level of funding. The next panelist thought that it would be better to run more tests with large format cells to further evaluate the proposed chemistries. In particular, this panelist recommended running abuse tolerance tests with a cell larger than the 18650 format cell. The final observer reported that the project had evaluated a number of methyl butyrate-based electrolytes in Conoco A12 Graphite/Toda HE5050LiNiCoMnO₂ three electrode cells (Argonne materials): The MB-based formulations containing LiBOB delivered the best rate capability at low temperatures, which was attributed to improved cathode kinetics. The final observer further reported that the use of lithium oxalate as an additive led to the highest reversible capacity and lower irreversible losses. The final observer further reported that at lower temperatures and higher rates, the advantages of utilizing the high voltage system diminished when

compared to a standard NCA material, again attributed to the relative cathode kinetics. The final observer concluded that, of the different cathodes, the LLC-NMC electrodes (received from Argonne) displayed much slower lithium de-intercalation kin.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? Three reviewers rated the resources to be sufficient, while one found them insufficient. One reviewer exclaimed that the value for money here was astonishing. This reviewer felt the project was obviously badly underfunded, and that the way forward was to either have the system replicated at a national laboratory or to increase the funding. Another panelist recommended identifying stable electrolyte systems for a 5V Li-ion cell at high and low temperatures-defined life-limiting mechanisms.

U.S. DEPARTMENT OF Energy Efficiency & Renewable Energy

Novel Phosphazene Compounds for Enhancing Electrolyte Stability and Safety of Lithium-ion Cells: Kevin Gering (Idaho National Laboratory) – es027

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments in this section were positive. One reviewer felt that, consistent with the DOE goals of reducing petroleum consumption and greenhouse gas emission by replacing the conventional automobiles with batterypowered hybrid and electric vehicles, this project addressed the safety of Li-ion cells by developing novel electrolyte solutions with reduced flammability and compatibility with high voltage (5V) cathodes, based on various phosphazene compounds. This reviewer noted that the current Li-ion battery electrolytes were flammable and thus played a significant role in the thermal runaway. This reviewer explained that phosphorus - containing compounds, specifically phosphazenes, on the other hand, were known to have reduced flammability. The reviewer further found that the objective here was to synthesize novel phosphazene based solvents that had good stability at high (5V cathode) voltages and high temperatures, and also formed desirable SEI characteristics on carbon anode on aging. Another observer stated that electrolyte



flammability was a major source of safety concern in current Li-ion systems. This observer felt that impacting this attribute would be quite relevant to battery adoption, especially in large format, mobile battery applications.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Reactions to this question tended to be negative. One reviewer thought that the approach was somewhat disjointed. This reviewer explained that the electrolyte approach seemed to focus on the flammability topic, albeit with somewhat marginal results, and that very little characterization of the flammability improvement was presented. This reviewer observed that the second topic of using the family of materials as an alternative anode may or may not be interesting, but in either case was not closely related to the topic, and completely unrelated to the task of developing a non-flammable electrolyte. Another panel member related that a high voltage stable electrolyte may improve the energy density of various Li-ion systems. This panel member reported that the concern with Ionic Liquid was low temperature performance (e.g. -30°C power capability). The final panelist characterized the adopted approach as based on the following: synthesizing and characterizing new phosphazene-based solvents with various functional groups in the pedant arm (i.e., ether groups, their unsaturated and fluorinated analogues, and even ionic liquids); performing DFT calculations for solvent-Li binding energies; and assessing their performance as electrolyte additives in Li-ion cells, especially those with ABR couples. This panelist found that there were considerable challenges here in terms of achieving desired interfacial stability at both the electrodes with the proposed solutions containing phosphazene additives, based on the earlier studies with the

phosphazenes as flame-retardant additives, which had not been quite successful. Nevertheless, this reviewer concluded that the project was well-designed and well-integrated with the other material development efforts under DOE, evident from the on-going tests with the ABR-relevant couples.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments in this section were mixed. One person considered flammability reduction through additive addition to be a very challenging approach to the issue. This person was not clear if the abuse results projected a significantly positive outcome. This person pointed out that there were a number of electrolyte level tests that could guide the direction of whether an electrolyte was showing improved flammability, but that these were not mentioned. This person concluded that the results from the effort to develop alternative material electrode material were too early for evaluation and would be complicated in development. Another panelist found that there was no low temperature performance data to meet USABC goals. The next reviewer decided that reasonable progress had been achieved here, and categorized that progress as follows: synthesized several new phosphazene compounds, especially fluorinated and ionic liquid substituted compounds; completed DFT calculations, which showed lower binding energy (with Li) upon increased fluorination; performed cyclic voltammetry studies that this reviewer emphasized did not support the argument of expanded voltage stability; carried out electrochemical assessment in coin cells with Toda HE5050/carbon couple, which showed the compatibility of electrolyte additives; and performed safety tests at SNL. This reviewer acknowledged that the safety tests at SNL showed slightly reduced heat rates in some cases, but noted that the effect was not significant because of low proportions of the additives. This observer felt that the electrochemical performance was difficult to judge because it was not normalized to the cathode capacity. The observer further considered the performance (mAh/g, and possibly voltage) of alternate anode materials being developed here based on phosphazene chemistry equally unclear. This observer recommended that the safety improvements from the phosphazene additives be demonstrated in conventional low-voltage systems to start with, rather than the 5V systems.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reaction to this question was mixed. One reviewer felt that there were good ongoing collaborations with ANL and SNL in the demonstration of the compatibility and safety with the phosphazene additives in advanced Li-ion chemistries being developed in the ABR program. This reviewer recommended some collaboration with universities that worked in the past on phosphazene compounds for similar applications.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments on this subject were generally negative. One observer still questioned if additives were a viable way to reach relevant flammability reduction levels. Another reviewer reported that future plans were to continue the synthesis of new phosphazene compounds with low binding energy with Li (from DFT studies) and evaluate them in coin cells with advanced ABR Li-ion couples for compatibility and electrochemical performance, and finally demonstrate their improved safety in 18650 cells from the abuse tests at SNL. This reviewer felt that the development of alternate anode materials based on this chemistry looked less attractive and feasible.

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

Two reviewers rated the resources excessive, while one found them sufficient. One panelist thought the resources were a little excessive for the project, based on the facts that the PI had several other tasks from ABR and the effort on alternate anode materials did not look as promising. Another panel member suggested that perhaps resources could be trimmed back a bit.

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Screening of Electrode Materials & Cell Chemistries and Streamlining Optimization of Electrodes: Wenquan Lu (Argonne National Laboratory) – es028

Reviewer Sample Size

This project was reviewed by five reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that the tasks were aligned with the overall objectives. A second person added that it was an important contribution to the overall DOE objectives because the research focus was not only on one electrode or problem but on the battery in general. The next reviewer said that the optimization and standardization of electrochemical testing was essential for a proper comparison of different projects within government labs. The next reviewer noted that, with several advanced materials of cathodes, anodes and electrolytes being developed in the ABR program as well as elsewhere, it was essential to have their performance independently assessed against the PHEV performance targets in standard test vehicles and environment. This person added that the objective of this project was to conduct independent screening tests using standardized test procedures to: streamline the lithium-ion electrode optimization process; enhance the understanding of these advanced materials; and select promising advanced materials and cell couples for an internal cell build and



further testing. By completing a successful verification, this project would serve as a bridge between the material development and the scale up/cell fabrication activities in the ABR program as well as lead to an infusion of the high-energy materials in PHEV cells and batteries, added the reviewer.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

One reviewer observed that the approach adopted here was quite similar to two other projects, ES029 and ES030, in the following ways: material characterization through XRD, SEM, EDAX, particle size distribution, etc.; optimization of electrode fabrication process; and cell fabrication and testing for electrochemical performance including reversible and irreversible capacities, ASI and cycle life; and thermal stability. Even though some additional work was performed in optimizing the electrode composition in terms of binder/conductive diluent contents, this project overlapped closely with individual material development projects as well as with ES029 and ES030, added the reviewer. The reviewer believed it to be redundant and thought that it was not critical to the material development and its infusion/demonstration in large cells. The reviewer continued, explaining that, like in some of the material development efforts, there appeared to be some disconnect and lack of coordination among the ABR/BATT projects, resulting in some duplication/redundancy, which would, hopefully, be eliminated in the upcoming restructuring of the ABR program. A second reviewer believed that this was a very important program that tested not only cathode powders. This person mentioned that it could be of interest to mention the tap density of the cathode powders being tested. The capacity unit that was
often used is mAh/g active material, and some of the values could be very impressive; however if the material did not load well, the powder may not have practical applications, added the reviewer. This reviewer also mentioned that failure analysis was also important, and could provide important information and suggest better electrode formulations. The next reviewer thought that the researchers had developed an overall good approach, but would have liked to have seen more attention given to high and low temperature performance as well as a slide showing the variability of cell performance to be assured this was minimal. The next reviewer felt that it was truly important to develop an effective and efficient tool to screen electrode materials and streamline optimization of the electrodes. It seemed that investigators had done a lot of work but added that it was difficult to understand the difference from what the industry did or to separate this work from the work of other groups within ANL. This reviewer suggested that needed to be tested, in addition to the routinely-tested properties; as well as include why the PI's approach to the optimization of the electrodes was streamlining. The final reviewer liked that the focus in recent times was going forward, unlike the focus in previous years, consisting of a variety of subjects.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first commentator to respond felt that, in general, the studies were of high quality, systematic, and well-presented. A second reviewer added that reasonably good progress had been achieved in evaluating several high energy couples and electrolyte formulations (with additives). The reviewer noted that some of the significant findings included the following: good rate capability and cycle life of 5V LMNO in carbonate-based electrolytes; high energy density from the ANL Li-excess composite 0.33Li₂MnO₃ • 0.67LiNi_{0.5}Mn_{0.5}O₂, but only at low rates and high states of charge; possibility of reducing binder/carbon content in cathodes; and good cycle life of Si-C cathode with a stable, approximately 450 mAh/g capacity in FEC-containing electrolytes, with little impedance gain. This expert added that some of the other miscellaneous studies included the study of redox shuttles, effect of carbon coating of Al, separator, and etc. These results were consistent with the findings from similar projects, without many new and significant findings, mentioned the reviewer. The third reviewer to comment stated that some of the measurements performed on batteries similar to commercially available ones were of great interest. At the moment, as indicated by the authors, the focus was on electrodes and cell fabrication, added the reviewer. The reviewer suggested that, at some point, it would be of great interest to design accelerated tests to study the failure mechanism of these batteries. It could be important, for example, to see if the Si composite anode changed the mechanism of failure of a battery, added the reviewer. Furthermore, since the authors have or would have access to practical batteries, it could be of great interest to report data in terms of mAh/g total electrode and not only in relation to the active material, suggested the reviewer. Another commentator believed that, since life was a very important issue with all Mn-based systems, the authors should have studied this aspect of the materials. The reviewer stated that Fluorinated Ethylene Carbonate (FEC) is known to have gassing/high temperature stability issues and suggested that this material be used in other similar studies. The last reviewer felt that there needed to be more emphasis on high temperature and low temperature testing and that a comparison with 5% carbon black would have been interesting.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer to respond felt that there was good collaboration across many groups having complimentary expertise. The second commentator said that, as expected from the nature of the project, there were several contributors and collaborators to provide electrolyte materials. A third reviewer explained that many people understood that it was not easy to collaborate and communicate with other institutions and that for obvious reasons companies usually preferred not to share technical information. This person wondered if at some point the project team may allow some disclosure of the data and asked if it would be possible to test commercial batteries and have the information shared with the companies involved in close door meetings. Another reviewer added that the screening of the industrial materials was desired and that it seemed that other groups within ANL were able to procure such materials. The final reviewer to comment believed that PIs, not just for this project, needed to talk to each other and take advantage of the talent pool as well as network with industry that ANL as a whole, has done.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer noted that the proposed future research was to continue the assessment of next generation materials from the Applied Battery Research (ABR) partners, external partners. The reviewer also mentioned that there were plans to study the voltage fade issue of the Li-excess layered composite materials, which was the focus of the ABR. A second reviewer thought the focus should be narrowed in on screening/improving key technologies that could bring significant improvements to the state-of-the-art; hence, focusing on composite-cathode or Si systems was okay. The reviewer added that the work on redox shuttles, binder, and etc. brought incremental improvements and should not have been funded. One reviewer suggested including additional work in their testing, including the use of high and low temperatures. Another reviewer observed that there had been a lot of progress and a variety of materials tested and hoped that the authors would engage more with battery manufacturers in the future. The final reviewer to comment felt that the future plans were inconsistent with the objectives of this project.

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

Three of the four reviewers to respond felt that the project resources were sufficient in order to achieve the project milestones in a timely fashion, while another reviewer felt that the resources were excessive. The first commenter to respond felt that the budget of \$750,000 (i.e., \$450,000 for screening and \$300,000 for optimization) looked a little excessive when the lack of significance and uniqueness of this project was considered. The second reviewer believed that there were probably not enough resources if the authors wanted to fully expand the cell fabrication capabilities. The reviewer further noted that the program seemed to be ending this year. A third reviewer expressed difficultly in assessing the project resources.

Scale-up and Testing of Advanced Materials from the BATT Program: Vince Battaglia (Lawrence Berkeley National Laboratory) – es029

Reviewer Sample Size

This project was reviewed by five reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

One reviewer stated that it was very relevant for the overall goal. Another reviewer elaborated, saying that it the overall objective of supported petroleum displacement by focusing on the mechanism of failure of electrolyte composition batteries. and additives, electrode fabrication and testing. A third reviewer explained that, with several advanced materials being developed in the BATT program, it was essential to have their performance independently assessed against the PHEV performance targets in standard test vehicles and environment. The reviewer stated that the objective of this project was to support the material development efforts in BATT by testing these materials as well as materials from industrial collaborators in half and full cells and comparing their performance to a baseline chemistry and thus identifying the failure modes. This person added that a successful verification would lead to further development of those materials in ABR or redirected research efforts under BATT. Another reviewer felt that it was important to have independent



evaluations to validate the performance of materials developed under the BATT program. The last reviewer believed the work to be relevant and expressed that other groups were doing similar tasks.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer to respond noted that the approach adopted here was to obtain new materials from BATT PIs and industrial collaborators, assess their key physical characteristics for particle size distribution, morphology and microstructure, and test their electrochemical reversible and irreversible capacities, and rate capability in half cells and full cells, and finally understand their performance-liming processes. The reviewer added that, even though individual PIs already assessed their own materials, this project would provide a standardized platform to assess the materials for proper comparison against the baseline and within themselves, and also to examine these materials in a system environment much like what ABR intended to do. A second reviewer observed that a lot of progress had been reported by the team, most of which was strongly focused on the voltage fade phenomena and the side reaction on the cathode on charge. These were critically important issues that had to be resolved for the potential implementation of those powders in the next generation of batteries. This reviewer suggested that authors should focus a little on trends; even if the absolute values may be off a little, they may provide trends to clearly show the strong and weak areas of different powders, separators, or electrolytes. The next reviewer felt that there was good focus on a number of materials but that the project could have been improved by focusing on materials of higher impact. The next reviewer to respond agreed that the

project was good, but thought that additional attention should have been paid to review the baseline observations. The reviewer thought the baseline results were strange (as shown in Slide 10 of the presentation) and suggested that the project leader use a second NCM from a different source and/or use a different baseline electrolyte. The best baseline electrolyte would have been from Daikin 1.2MLiPF₆ in FEC/EMC, added the reviewer; furthermore, the use of standard Novolyte was not recommended for use at 4.5V. The next responding reviewer believed that it was important to have independent evaluations to validate the performance of materials developed under the BATT program. However, it was more important to develop testing procedures focused on identifying the sources of failure and having a feedback mechanism in place to help the PIs improve/modify their materials, added the reviewer. The next reviewer wondered how the materials were being selected for testing under this project. Another question brought forth by a different reviewer was whether there were protocols that were consistently used or if each PI provided the best procedure for the material to be tested.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer to respond stated that the project had evaluated a considerable amount of new materials potentially useful to the overall DOE goals and added that the database was quite useful. The second reviewer felt that good progress had been accomplished in terms of evaluating several BATT samples and external (industrial) materials, which included NMC333 and LMNO (Ni-substituted manganese spinel oxides) cathodes in different electrolytes (three high voltage electrolytes) containing proprietary co-solvents, additives or salts. The reviewer found the effects of electrolyte on the irreversible capacity (side reactions), and of cathode on the anode impedance to be very interesting. This person added that some combinations (for example, the MIT cathode with FEC-containing electrolyte and CGP-G8) appeared to be quite good in terms of capacity retention and the effects of such electrolyte variations on the individual electrodes as well as the effects of cathode on the anode impedance would be better understood with three-electrode cells. The next reviewer explained that a variety of tests were implemented and suggested that it could be of interest if in the future some data was presented in relation to the mechanism of failure (for different cathode powders, for example). As mentioned by the author, measurements with a reference electrode (which are not easy to do) may give important new insights, added the expert. The next two reviewers agreed that the project showed a good in-depth analysis of the observed results. One reviewer added that much of this explanation may not have been needed if changes to the approach had been implemented. Another reviewer added that it would be desirable to see more effort spent on testing that was beyond what industry could do to take advantage of the unique instrumentation base of the national laboratories. The first reviewer recommended having the laboratory be able to evaluate the materials at high temperatures (say 50° C) so that the life aspects of the materials could be looked at. Mere room temperature work does not tell the true story, added the reviewer. The reviewer had heard many times within these programs that this or that material (and many of them) looked very promising, but never heard about them anymore. The second reviewer was unsure what the next step would be with the successful electrode/electrolyte combinations identified here. The reviewer asked whether there was any plan to demonstrate their enhanced performance in prototype cells with industrial battery manufacturers or if they would be absorbed in ABR. The last reviewer to respond felt that it would be interesting to know the correlation between doping/coating approaches versus electrolyte/additives approach to mitigate interface reactions on both positive and negative sides.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer felt that it seemed like the team managed to build a strong collaboration with different institutions and companies. The next two reviewers added that there were a good number of extensive collaborations with well-known researchers and companies. Another commentator stated that, as expected from the nature of the project, there were several contributors and collaborators providing electrode electrolyte materials. This reviewer added that the project would probably benefit more from some collaborations with an industrial battery manufacturer in scaling up/verifying these materials. The last reviewer to respond asked if the feedback loop existed to help partners improve on their products, and suggested that it would be great to see an example presented next year.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer felt that this project provided an excellent channel for many researchers to get their materials evaluated per advanced testing protocols. This reviewer believed that the bulk of the focus should be on high impact materials such as the next generation cathodes and anodes that could bring costs down significantly or make the cells abuse-tolerant. The same reviewer opined that topics such as binder and use of electrolyte additives only brought about incremental improvements to cell performance and should not receive focus. The following reviewer noted that the proposed future research included: continuing the assessment of next generation materials from the partners; seeking correlations between performance and electrode/electrolyte properties; working towards scaling up the LMNO cathode; and carrying out three electrode measurements to better understand the anode impedance rise. This person added that there were plans, consistent with the program goals, to develop proposals to the next phase of ABR on the same concept. The next reviewer noted that the project was ending this year. This reviewer suggested continuing the future research with the good communication the project team had developed with partners and industry. Analysis of batteries at the end of life should also be considered, added the reviewer. The next reviewer suggested getting an appropriate baseline electrolyte from Daikin 1.2MLiPF₆ in FEC/EMC, or requesting a similar formulation from Novolyte. The last reviewer to respond stated that the PI clearly showed an understanding of the issues and the path forward and had addressed them during the oral presentation.

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

All four reviewers felt that the project resources were sufficient in order to achieve the project milestones in a timely fashion. The first reviewer to respond considered the importance of the project and supported increasing its funding. Another reviewer felt that the budget looked adequate; if not slightly lower, for these studies. A third commentator believed that the resources were sufficient; however, the expert added that it was hard to know since the project was finishing. This person added that the authors had done a great job based on the amount of resources they received. The last reviewer felt that this was a difficult question to answer. This person suggested increasing this project's resources in order to provide independent testing for all BATT-funded materials.

Fabricate PHEV Cells for Testing & Diagnostics: Andrew Jansen (Argonne National Laboratory) – es030

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer noted that this project covered the cell level test for material evaluation. Another reviewer felt that it was important to get a measure of material capability in finished cells which were well sealed. This reviewer also noted that this facility allowed experimentation on mix formulation, mixing conditions as well as material sources in validated cells.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? One reviewer felt that this group was making a dedicated effort to bring the facility into operation and replicating the manufacture of sealed cells utilizing pilot line equipment. Another reviewer felt that if the validation was successful, runs with test materials would be much more useful to material developers. A third reviewer noted that the cell design and validation lacked the development for the standard cathode for the anode evaluation, respectively. This reviewer expected other



material companies to get the benefits from this testing facility as well as ANL-developed material does (DOE-funded cathode, anode, electrolyte and separator developers). The last reviewer added that, while several details were lacking in the presentation, it appeared that a full evaluation of the equipment had not yet been carried out. The reviewer suggested that a material in current production such as LCO, LMO or NMC cathode material should be utilized with a common formulation for that material used in industrial cell making. This person added that the coater should be tested for uniform loading from side to side and from front to back by sampling either with simple punching and weighing of samples after drying or by the use of a beta gauge to determine loading in real time. The electrodes should then be made into cells of both cylindrical and pouch types to test assembly methods, added the reviewer. The reviewer also believed that the performance after standard formation should be measured appropriate to the electrode and cell designs and then compared to comparable production cells, after the standard electrolyte fill was validated.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer to respond felt that the accomplishments were good in the sense of setting up an entire pilot line production facility. The reviewer added that there was a lot of validation required (as noted above), however. The reviewer believed that the group should focus on this matter before launching new material assessment as there would always be questions regarding the accuracy of the cells as made. Another reviewer did not think that the SOP and quality criteria for each assembly process step were set up yet. This person also noted that the capability of 18650 cells was also not yet set up.

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Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

One reviewer felt that the project needed to get help from the company for setting up the SOP and pass criteria for each step of process. Another reviewer suggested working with a consultant with cell-making experience to assist in the validation work and in the accurate alignment of all the machines. Coaters, winders, pouch cell placers and other equipment all required accurate settings which should be tested regularly, added the reviewer. This person stated that this work would result in SOPs that would assure a quality product.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer felt that this facility should be more open to DOE-funded materials companies.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? Two of the three reviewers felt that the project resources were sufficient to achieve the project milestones in a timely fashion. One reviewer felt that the resources were insufficient. Another reviewer suggested hiring operators for a higher production capability.

Electrochemistry Cell Model: Kevin Gallagher (Argonne National Laboratory) – es031

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer to respond felt that modeling may provide insights regarding battery performance and the mechanisms for degradation that are unobtainable through experimental methods while another reviewer suggested that the team should focus on the important issues.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? One commentator noted that the approach was to link experimental work with the developed electrochemical model to identify performance limitations and aging mechanisms. The next reviewer stated that by homogenizing all material properties, any degradation due to local inhomogeneity would be automatically ignored. The last reviewer to respond suggested using better input parameters when applying the Newman model to the positive electrode. This person asked what else was different and new.



Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer to respond stated that the studies of aged electrodes were good, but added that this sort of approach had been used for many years. A second reviewer felt that the model indicated that the most likely source of impedance growth (i.e., interfacial contact resistance between LMR-NMC particles and the conducting carbon additive) occurred in the cell upon aging. The electrolyte parameters were supplied by Kevin Gering's Advanced Electrolyte Model, added the reviewer. This reviewer wondered if this information had been (at least partially) experimentally validated and noted that the model was now being used as part of the effort to understand the open-circuit voltage (OCV) fade of the cathode upon aging. Some hypotheses have been suggested for the OCV hysteresis including two sets of vacancies (sites) or reversible structure change, added the reviewer. The reviewer felt that another potential difficulty noted by the model and this work was that the lithium diffusion coefficient in LMR-NMC was much lower than for NMC, but one is unsure of the reason for this. The reviewer asked how the results from the modeling work would be validated experimentally to confirm their accuracy. The next commentator observed that the project had used (ANL's) Dennis Dees' physical model to interpret impedance and believed that there was no statistical significance or cross correlation information. The next reviewer to respond found it interesting that the hysteresis depended strongly on the voltage, but was also unsure of the explanation. The reviewer added that the hysteresis depended strongly on the voltage, but with all of the micro-scale information now available, future models should go beyond homogenized material properties.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The only reviewer to respond noted that collaboration included working with Daniel Abraham and Andrew Jansen (among others) at ARL and Kevin Gering at INL. This person added that more collaboration would be established from the PIs' participation with the voltage-fade team.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer noted that the future work would include participation in the team of researchers examining the problems of voltage fade and the refinement of the negative electrode SEI growth model. The next reviewer was unsure how this level of modeling could contribute. The reviewer added that Newman's model had always been very successful in modeling battery performance, but not so with degradation. This person explained that people have made *ad hoc* patches to the model and fit coefficients of additional terms to reproduce the degradation data, but added that this was hardly predictive. The last reviewer to respond suggested that a more selective focus on materials-specific topics would be helpful.

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

Three of the four reviewers to respond felt that the project resources were sufficient, while another noted that the resources were insufficient. The first reviewer felt that there were sufficient resources, which appeared to be available for the proposed work. This person added that it was difficult to gauge this without a full budget. A second reviewer stated that a much larger effort would be required to go beyond Newman's homogenous approach.

Diagnostic Studies on Lithium Battery Cells and Cell Components: Dan Abraham (Argonne National Laboratory) – es032

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

One reviewer described that the project involved advancing the general understanding of degradation mechanisms in Li-ion chemistries. Another person simply stated that high energy couples were of high relevance. The final reviewer acknowledged that diagnostics facilitated the identification of mechanisms and challenges at the material, electrode, cell, and battery pack level. Such studies were crucial and should be pursued in parallel with material, cell and pack development. In some instances, the diagnostics provided key information about widely-recognized problems. In other instances, however, the reviewer cautioned that the diagnostics studies indicated potential problems/difficulties of which researchers may be unaware thus pointing to new research directions.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project welldesigned, feasible, and integrated with other efforts? Reactions to this question were mixed. One person described that the approach was to identify the causes



(either materials or mechanisms) responsible for cell performance and degradation in performance through the use of advanced characterization tools. Another evaluator explained that the approach included the disassembly of new and aged cells and analysis with a very wide range of diagnostics. The reviewer added that the use of reference electrode cells was vital, and not everyone did that. The reviewer did not see how the TEM and XPS analysis/diagnostics results could be converted, even in principle, to specific, actionable recommendations to the rest of the team. The final reviewer commented that the approach to this project's work was generally good but could easily be farther-reaching.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

All responses to this question were positive. One person remarked that the project had a number of accomplishments which may be ground-breaking and of great value towards advancement of Li-ion battery technology, while at the same there were a number of accomplishments which could be easily arrived at within typical industry activities or by a large number of less well-equipped and less well-funded institutions. Another reviewer pointed out that the researchers determined that the upper cut-off voltage was an important determinant of the ABR cell life, which is important, but is already known. The reviewer added that what was new was that the oxide-carbon contact was where the problem was. The reviewer also highlighted that the cross-talk between electrodes and the fact that the positive electrode impedance rose was the common feature in all couples were both important and new. The reviewer felt the recommendations were good, but some, such as the additives and coatings could be helpful, were already well

known. The reviewer would have liked to see the researchers make an attempt to take advantage of the new knowledge about the oxide-carbon interface. The final reviewer had detailed comments, describing that the researchers: concluded studies of PHEV baseline materials (NCA/graphite); began characterization and aging experiments on electrodes and cells for new materials; and concluded that electrolyte oxidation at the positive electrode contributed significantly to the impedance rise and that lithium trapping in the negative electrode SEI was the main contributor to the cell capacity fade (not the cathode, or at least not directly). The reviewer reported that possible solutions included positive electrode reformulations (altering carbon and binder contents, mixing procedures, and calendaring conditions) to reduce impedance, electrolyte additives, and positive electrode coatings (i.e., Al₂O₃). The reviewer highlighted that the use of reference electrodes for the full cells was demonstrated to be very informative for this work. The reviewer offered one critique – that very little of the crucial diagnostic information (i.e., performance degradation) obtained from the work associated with this project has been published in open, easily-accessible scientific literature. The reviewer concluded by explaining that such information would be very much welcomed by the battery research community because there was very little of it available at this time.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reactions to this question were positive. One person mentioned that numerous organizations were listed as partners for this project and that the characterization work was distributed throughout these institutions, although the bulk of it seemed to occur at ANL. The other person to comment expressed that the collaboration was excellent for universities and national laboratories. The reviewer pointed out that adding battery or chemical companies would make the collaborations even better.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reactions to this question were mixed. One person felt that this part of the talk was quite vague. While another person described that future work would include the continuation of the evaluation of the ABR-1 electrochemical couple and cell constituents, initiation of work associated with the next set of ABR couples and work linked to the voltage fade for LMR-NMR oxides. The reviewer added that all were worthy of pursuit in order to advance the DOE's goals.

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

Reactions to this question were mixed, with two reviewers stating that the resources were sufficient while one thought they were excessive. One person added that the project appeared to be well-funded and that ANL was well-suited in terms of resources for this project. The other reviewer to comment observed that almost every possible diagnostic technique was available to this team.

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Electrochemistry Diagnostics of Baseline and New Materials: Robert Kostecki (Lawrence Berkeley National Laboratory) – es033

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reactions to this question were all positive. One person commented that the project activity identified key Li-ion degradation mechanisms battery using unique applications of diagnostic methods. The reviewer added that this project provided a pioneering illumination of the opportunity paths for improved Li-ion battery performance, and that these paths were unlikely to be so usefully identified by any other research entity within the U.S. in the near future. Another reviewer described that the project included high cell capacity, degradation, and SEI formation; which includes most of everything that is important. The last reviewer provided detailed comments explaining that diagnostics facilitate the identification of mechanisms and challenges at the material, electrode, cell, and battery pack levels. Such studies were crucial and should be pursued in parallel with material, cell and pack development. In some instances, the diagnostics provided key information about widely recognized problems; in other instances, however, the diagnostic studies indicated potential



problems/difficulties of which researchers may be unaware thus pointing to new research directions. The reviewer concluded by stating that degradation was, of course, one essential area of research to meet the high demands required from batteries for traction applications.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

All responses in this section were positive. One person commented that the focus of the purpose and scope, and the targeted approach of the crosstalk studies, and the carbon black (CB) additives studies were outstanding and should be seen as models for the Advanced Battery Research for Transportation (ABRT) activity in general. Another reviewer felt that it was good that the project team went beyond determining mechanisms to investigating mitigating treatments, and that post-test diagnostics were good. Researchers applied new diagnostic techniques to the battery field, especially *in situ*. This reviewer felt that it was very important that the author showed micro-scale inhomogeneity, which may be the ultimate source of most degradation, and added that very few studies recognized, let alone analyze inhomogeneity. The reviewer really liked that researchers designed unique cells to get answers, for example making electrodes just out of CB. The reviewer also considered it very good to model the experimental results. The last panel member characterized the research as: having examined the impact of high potentials on the carbon black added to cathodes; having determined the key factors that contribute to the component and cell degradation (PHEV couples); and having characterized SEI formation on model electrode surfaces to improve the understanding of the interfacial phenomena.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Responses to this question were generally positive. One reviewer felt the accomplishments of this project were outstanding and should be viewed as among key highlights in the entire ABRT program. Another panel member considered analysis of carbon black additives important and the new information on mechanism of CB very nice. This panel member thought it was really great that the researchers identified an approach to solving problems that could work at industrial scale CO₂. The panel member stated that fluorescence analysis needed to be connected to performance, and thought it was very important to demonstrate that carbon blacks were electrochemically active, even allowing PF_6 intercalation. The final observer pointed out that although the use of fluorescence imaging to detect electrolyte decomposition was demonstrated, no mention was made regarding controls. This observer questioned what the comparable data was if the same cells were cycled to a lower voltage. Further, the observer questioned what the influence of additives or surface layers was, and stated that it seemed that only a limited amount of work was done. It was determined that the degradation products from the cathode affect the anode (SEI layer) and the side reactions producing these products may affect lithium availability (inventory). In particular, the anion may intercalate into carbons leading to degradation (as reported during the last year). A surface treatment with CO_2 was demonstrated to reduce this phenomenon. This observer was unclear if it was therefore deemed crucial to modify the baseline high-voltage cathodes currently being tested as part of the BATT program with treated carbon. The observer went on to question if this information was being applied to improve the work of other battery research, and pointed out that most of the work had been disseminated in presentations rather than in widely available scientific publications. The observer concluded that, given the importance of this work, it was desirable that the work be published in one or more prominent battery research-related journals.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments on this section were mixed. One reviewer saw good collaboration among national laboratories, but suggested that it would be better if it also included universities and industry. Another reviewer acknowledged that the significant challenge of collaboration from within the ABRT programs with international institutions and/or international industrial partners could not be underestimated, but suggested that this would be one key area for potential future expansion of utility of outstanding projects such as this one. The final reviewer thought that LBNL seemed to work closely with ANL and BNL, both in terms of cell preparation (at ANL) and characterization, but that it was not clear from the work presented what, if any, of the work was done through collaborations this past year. There was a note on Slide 5 that indicated that no test cells had been sent to LBNL in FY 2011 and FY 2012. This reviewer questioned what the significance of this was, and what work, if any, had been done in conjunction with companies to facilitate their diagnostic needs for high-voltage electrodes.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reactions to this question were positive. One person found that the aims were related directly to end use, which is better than if they were just aimed at understanding. This person thought that the planned future work would lead directly to achieving DOE objectives. Another reviewer suggested that a further study of a wider variety of CB additives and treatments could be beneficial. The final observer reported that the proposed future work would continue searching for a means of decreasing the irreversible capacity losses during cycling through surface treatments. Post-test characterization would be performed on ABRT cells to examine electrode composition, structure and surface films. Work would continue to examine the degradation mechanisms in cells. This observer felt that there was no indication of what specific additional testing would be done or what new materials would be studied.

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

All three reviewers found resources to be sufficient. One felt that all required resources were available, and another stated that the funding seemed to be quite high (\$600,000) based upon the amount of work reported, but perhaps that other work had been performed as part of this project that was not reported.

Diagnostic Studies to Improve Abuse Tolerance and Life of Li-ion Batteries: Xiao-Qing Yang (Brookhaven National Laboratory) – es034

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments for this section were generally positive. One reviewer felt that this work provided useful insight in many fundamental mechanisms involved with a number of important materials of interest to vehicle electrification in industry. Another person thought that projects reducing costs were especially valuable, and that understanding failure was good. The last reviewer explained that diagnostics facilitated the identification of mechanisms and challenges at the material, electrode, cell and battery pack level. This reviewer felt that such studies were crucial and should be pursued in parallel with material, cell and pack development. In some instances, the diagnostics provided key information about widely recognized problems. In other instances, however, the diagnostics studies indicated potential problems/difficulties of which researchers may be unaware, thus pointing to new research directions.

Question 2: What is your assessment of the approach to performing the work? To what degree

transformations upon cycling.



are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Reactions in this section were generally positive. One panelist felt that the project made excellent and creative use of BNL's relatively unique equipment and experience capabilities. This panelist also thought that the choice of materials to be studied was understandable from a DOE perspective but that the materials could be improved if the automotive industry and its real-world applications were of prime importance. Another observer reported that the overall approach was to make structural measurements on materials of interest. The final reviewer observed that this project utilized time-resolved x-ray diffraction (TR XRD) and mass spectrometry, together with XAS (XANES and EXAFS) and TEM to examine the thermal stability of electrode materials. Cathode materials had been surface modified with ALD, whereupon the materials (LMR-NCM) with and without the coatings were studied to determine the voltage and capacity fading mechanisms. This reviewer concluded that it was evident from the work presented that a lot of insight was gained from the methods used into the mechanisms for thermal degradation, as well as material

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Commentary on this question was mostly positive. One observer reported that a new *in situ* technique was developed in which TR-XRD was combined with mass spectrometry. The thermal stability (phase changes, gas loss, etc.) of different electrode materials was then analyzed with increasing temperature to determine the mechanisms of thermal degradation. This observer thought that

using the two methods in concert was extremely helpful, and that the use of XAS to aid in deconvoluting the origin of the voltage drop seemed to be very informative as it pointed to slowly evolving structural transformations. Finally, this observer remarked that the methods used provided key information about the role of surface coatings on stabilizing the electrodes. Another reviewer observed good progress towards project-specific goals. The final panelist pointed out that although new diagnostic techniques were developed, and these studies provided a new understanding, the project team needed to show how the project led in some way to ideas that would produce solutions. The panelist questioned, for example, what new information was obtained from the oxygen evolution experiments that was not already known. The panelist similarly questioned if measuring bond length and local structure helped solve problems, and if so, which ones, and how. The final panelist did not see progress towards the barriers that were supposed to be addressed.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reaction to this section was mixed. One reviewer felt that overall level and nature of collaboration was excellent. Another observer characterized that collaboration was extensive, with a diverse range of national laboratories, universities and companies. A different reviewer found that this project was unusual in having industry, laboratory, and universities. This reviewer thought that this project needed better coordination with the rest of the ABR program; i.e., these diagnostic techniques needed to be employed in a more targeted way, rather than answering vague questions. This reviewer suspected that there were connections, but they were not made clear. The reviewer concluded by suggesting that this project belonged in BATT or BES. One of the panel members noted that collaboration with a single automotive OEM on this specific topic was conspicuous and of concern.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments for this section were mixed. One person thought that expanding collaborations, including with industry, was good. Another panelist urged researchers to continue and expand upon the existing work. The final reviewer felt that the choice of materials to be studied in future research could be improved to better reflect automotive industry as a whole.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? All three reviewers rated resources to be sufficient. One thought that the funding was relatively modest for this project relative to the information gained.

U.S. DEPARTMENT OF ENERGY Energy Efficiency & Renewable Energy

Develop and Evaluate Materials and Additives that Enhance Thermal and Zonghai Chen (A

Additives that Enhance Thermal and Overcharge Abuse: Zonghai Chen (Argonne National Laboratory) – es035

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments for this section were positive. One reviewer stated that the role of safety performance in the commercialization scheme of Li-ion batteries was a critical factor in the potential adoption curve. Another panel member found that if the development of overcharge protection or prevention was successful, that would simplify the BMS and reduce the cost of the energy systems. The final reviewer reported that Li-ion cells could pose safety problems (thermal runaway) upon electrical or thermal abuse attributed to the thermal instability of the materials. These problems were somewhat aggravated with the advanced cathode and anode materials being developed for the PHEVs. The objective of this project is to identify contributions from each of the cell components of different chemistries to the abuse characteristics, and utilize this understanding to develop new abuse-tolerant materials and provide them to SNL for validation of safety benefits in 18650 cells. This reviewer concluded that it was essential to improve the safety characters of Li-ion batteries for



them to be used in widespread applications, such as PHEVs and EVs.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Reactions to this question were mixed. One reviewer explained that the approach targeted improvements in all the cell components for increased safety, e.g., safer anodes and cathodes, additives for stable SEI, surface modification for cathode, safer electrolyte components (solvents and salt) and redox shuttles for overcharge protection. Materials were being obtained from in-house researchers, external partners and commercial sources and assessed for electrical performance as well as safety improvements, which were subsequently verified in 18650 cells. The thermal stability of the cathode materials had been particular addressed here with and without the electrolyte components and using *in situ* High Energy XRD for understanding the evolution of new phases upon heating. This reviewer believed that this approach was very similar to another project ES 37 (Yang et al), where more comprehensive studies were being carried out and that there should be some coordination between these two projects. The reviewer concluded that the approaches looked reasonable and feasible and would lead to a further understanding of safety issues of each components and their potential for heat release, and thought the *in situ* measurements would be beneficial. The final reviewer wrote that the examples given of technical accomplishments did not suggest a coordinated approach to the issue of individual material safety considerations; in other words, a bit of a hodge-podge of areas was under investigation. The reviewer

admitted, however, that the single detailed example was comprehensive in nature and represented quite an interesting investigation.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments for this section were positive. One panel member thought the technique for development of High Energy X-ray Diffraction used in the following cell reactivity was quite an interesting accomplishment. The validation of the technique was not presented in detail, but this panel member hoped this had been investigated fully in terms of reliability, accuracy and repeatability as it could become an important technique which would produce good information. The other observer reported that reasonably good progress had been accomplished in terms of evaluating various cathode materials for their structural changes during electrochemical cycling and thermal abuse. Specific accomplishments noted by this reviewer included the following: *in situ* HEXRD study on charged $Li_xNi_{0.9}Co_{0.1}O_2$ with and without gradient composition, and $Li_xNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ cathode materials during heating; confirmation of the poor reproducibility of DSC data for delithiated cathodes; and investigation of the effect of salts (LiPF₆ LiBF₄, LiTFSI and Li₂B₁₂F₁₂) as well as pure solvents on safety. This reviewer found it interesting that LiPF₆ reduced the onset temperature from approximately 310°C to about 200°C as compared to other salts. This observer also pointed out that studies were ongoing on the ANL redox additive as well as on amorphous carbon covered graphite from Superior Graphite. The reviewer concluded that all these studies were matched the overall goals, but their significance was not clear yet.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Responses were neutral for this section. One reviewer reported that there is some collaboration within ANL and with external partners. The other reviewer stated that the project had planned to re-scope to merge with voltage decay project.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reactions to this question were somewhat positive. One reviewer repeated that re-scoping to merge with voltage decay project was planned. Another panelist concurred that consistent with the increased emphasis in ABR for the voltage slump in the LMR-NMC cathode, future efforts would be rebalanced between the safety and the voltage fade of lithium-manganese-rich NMC materials. Specifically, these studies were aimed at investigating the structural evolution of LMR-NMC during and after electrochemical activation using synchrotron-based *in situ* techniques. Also, the effects of surface chemistry on the SEI over carbon anode its thermal stability would be examined. This panelist found the planned studies helpful in mitigating the technical barriers of safety and increased energy density for Li-ion cells. The final reviewer believed that full development and evaluation of the technique of HEXRD should be pursued as a technique development capable of being accessed by the wider community.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? Two reviewers found resources to be sufficient, while another one found them excessive. One person repeated that re-scoping to

merge with voltage decay project was planned. Another thought that the budget of \$500,000 per year looked quite slightly excessive for this effort.

U.S. DEPARTMENT OF ENERGY Renewable Energy

2012 Annual Merit Review, Vehicle Technologies Program

Evaluation of Abuse Tolerance Improvements: Chris Orendorff (Sandia National Laboratories) – es036

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer said that this project was one of the important programs because it ensured the safety of Liion cells and batteries. The second reviewer felt that this project would provide a good tool for the selection of safer and cost-effective materials. Safety of batteries was definitely an important factor for realization of a broad adoption of Li-ion batteries for electric vehicles and overall DOE objectives. Higher energy batteries without the right and multiple safety protections might cause an unacceptable number of incidents. Using inherently safe materials was the most reliable protection method. Another reviewer stated that issues related to the safety of Li-ion cells which were identified and probed through the SNL's abuse tolerance studies needed to be solved in order to promote the mass commercialization of plug-in electric vehicle technologies. In addition, the same reviewer commented that an increased market share of plug-in EVs in the U.S. would lead to petroleum displacement.

Question 2: What is your assessment of the approach to performing the work? To what degree



are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer said that the Orendorff group (at SNL) had an extensive program addressing many aspects of abuse tolerance in Li-ion batteries and provided numerous sets of data to support this. Another reviewer stated that to evaluate the safety of batteries with 18650 cells was a legitimate approach. Additionally, comparing various technologies by using the same equipment and conditions was also a vital and convincing approach. This reviewer acknowledged that the goal of new electrolyte development, especially Ionic Liquid, was rather aggressive and cause for concern regarding dilution of effort. On the other hand, continued this reviewer, toxicity of gases generated from thermal abuse condition should be evaluated in addition to flammability of batteries. The same reviewer added that at least decomposition materials erupted from cells during abuse tests needed to be analyzed as this analysis would also provide insights for the degradation process mechanism.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

In general the testing was commended by the reviewers. The first reviewer stated that great progress was demonstrated for a quantitative evaluation method (isothermal calorimetry) with 18650 cells, including establishment of the fabrication capability and further noted that this method was broadly applicable to other new materials development. In addition, the results of RS2 were impressive as the effect of RS2 was clearly demonstrated and its limitation for higher current was quantified. The first reviewer also observed very good validation of the concept for LiF/ABA. The second reviewer said that it was clear that the test capability

was set up well to what was wanted, while the safety test could be done combined with the gas analysis tool including the cell fabrication. The final reviewer stated that the measurements conducted in this lab supported investigations of materials created in collaborating labs. Additionally, this reviewer felt that while there did not seem to be a major breakthrough in this batch of results, the research approach and data sets seemed solid and thorough.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated that collaborations to obtain various materials were well planned and performed, though there may be room for further collaboration regarding analysis for decomposed gases and cells after abuse tests, such as with ANL. The second reviewer felt that the Orendorff lab appeared to be the go-to place for other national laboratories to understand how batteries and their constituent materials could be made to withstand expected abuse conditions. Furthermore, its relationship with these other groups was symbiotic, resulting in the need for deep collaboration. The final reviewer suggested that the DOE team consider how it can deliver its knowledge to cell developers and manufacturers in the United States.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer felt that all remaining milestones and future plans described were reasonable. For the remaining project years, this reviewer requested that a specific plan be presented to understand the mechanism explaining why the non-HF generating electrolyte does not give runaway type decomposition while the LiPF₆ electrolyte does on the thermal abuse test. With that, continued this reviewer, material selection of ABA would be performed more logically. The same reviewer asserted that in addition to overcharge and thermal abuse, other failure modes should be analyzed and their priorities should be considered. Additionally, although no specific plan was described and the reviewer was uncertain whether these were planned, mechanical abuse and nail penetration tests were example areas of concern from a safety perspective. The second reviewer said that the researchers were looking at the results from the current studies to give direction to the next steps in the various projects in which these laboratory studies played a role.

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

All reviewers agreed that the funding resources were sufficient. The first reviewer observed that after establishing equipment and its protocol, rearrangement of the budget would be required for the next fiscal year. This reviewer further stated that the current budget level should be sufficient to further expand the types of abuse tests, and that the budget was not excessive. The second reviewer said the activities in the laboratory seemed congruent with the level of funding.

Overcharge Protection for PHEV Batteries: Guoying Chen (Lawrence Berkeley National Laboratory) – es037

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that if the development of the overcharge protection was successful, then it would simplify the BMS and reduce cost of the systems. The second reviewer described that Li-ion cells were intolerant to overcharge, unlike the aqueous rechargeable system, which may lead to either reduced cycle life or more importantly a thermal runaway. Li-ion cells were thus required to be well-matched to start with, and further, protected and balanced during cycling using sophisticated electronics. Attempts to achieve built-in overcharge protection though redox shuttle have not been quite successful yet, due to limitations from the solubility, diffusivity and compatibility of the redox species. The objective of this program was to develop a reliable, inexpensive overcharge protection system using electro-active polymer for internal, self-actuating protection. Improvement in safety and enhancement in cycle life were crucial requirements for the widespread use of Li-ion batteries in PHEVs. The third reviewer indicated a reserved yes. Overcharge protection on the individual cell level would be of some advantage to pack level safety and even performance. As noted, there were



competing approaches (electronic, shuttle) that this approach would need to be compared with. Ultimately, the reviewer was not sure this was the highest priority issue being faced. On the other hand, this was not a highly funded effort so the value was not out of line.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer stated that the approach seemed well thought out and logical, within the scope of the program. The first reviewer suggested that while at this stage the development was quite fundamental, that it would be prudent to establish some level of success criteria on a commercial level to make sure that competing approaches did not hold some unobtainable cost or processing advantage. The second reviewer stated that the approach sounded interesting and overall, was feasible and quite relevant to the activities of ABR. The reviewer summarized the approach in several statements that followed. The approach focused on developing electro-active polymers that could switch from a non-conducting to conducting state at potentials slightly higher than the cathode charge potential. The conductivity in the polymer changes by several orders of magnitude and the changes were fairly rapid and reversible and the cell voltage regulated the resistivity of the polymer shunt (e.g., polythiophene). Such a polymer layer could be placed in series or parallel to the anode and cathode stack, which would provide a bypass or shunt for the charge current. In cases where the polymers did not have the oxidative or reductive stability, a bilayer arrangement was adopted with individual high-voltage and low-voltage polymers for the cathode and anode side, respectively. However, due to the polymer sandwiched

between or shunted across the anode and cathode, there would be some enhanced self-discharge through this polymer. Also, the energy efficiency in the absence of overcharge would be reduced by this polymer switching. Possibly having the polymer from conducting to non-conducting phase (like PTC in 18650 cell) and have one for the anode to prevent lithium plating would be interesting options here. The last reviewer said that the use of self-discharging conductive polymer may not interfere with the cell chemistry.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer said good progress had been accomplished in terms of: identifying an electro-active polymer (PFOP) with an extended stability to 4.25 V (its stability at the anode appears to be poor), which was tested against three cathodes (LiFePO₄, NMC₃₃₃ and 4V spinel oxide); modifying the electroactive polymer to increase the sustainable current density; developing process for preparing the electro-active polymer-fibers and their composite mats were prepared by an electro-spinning technique; and characterizing the behavior of the fibers as charge carriers in Li-ion batteries in an *in situ* optical cell. In addition, this reviewer stated that a more comprehensive set of performance data, for example on the ASI and power densities of the cells with such electroactive polymer as a function of state of charge, the penalty in energy efficiency etc., are to be assessed to establish the viability and feasibility of this approach for overcharge protection. The second reviewer felt that technical data at the cell level was quite interesting and suggested that it would be important to characterize the physical handling properties of the material if it was contemplated to be inserted as a separator material replacement.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated there was some useful collaboration within LBL and with external partners on polymer synthesis. Collaboration with a battery manufacturer, to demonstrate these materials in an 18650 cell for instance, would be beneficial at a later stage. The second reviewer agreed that collaboration with a cell developer would add to the value of the project.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The reviewer stated that future studies involved continuing efforts to: demonstrate the benefit of such electroactive polymers in cells; examine other modes of deploying the polymer within the cell; develop high voltage electroactive polymers for lithium-excess high voltage cathodes; and scale up the effort through industrial partners. The reviewer felt that these studies were well directed towards the project goal of providing efficient and low-cost overcharge protection for Li-ion cells.

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

All of the reviewers agreed that the project funding was sufficient. The first reviewer stated that the budget looked reasonable for this effort. The second reviewer was in agreement and stated this was a very academic environment right now, which was fine for this current stage. This reviewer suggested that if the project were to receive any significant commercial interest that it would need to move up through the system to a more commercially focused area. Finally, this reviewer noted that this was a modestly funded area (correctly so) and the work had shown good use of these modest resources.

Inexpensive, Nonfluorinated (or Partially Fluorinated) Anions for Lithium Salts and Ionic Liquids for Lithium Battery Electrolytes: Wesley Henderson (North Carolina State University) – es057

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer felt that this approach showed promise and stated that for improved cell performance a new electrolyte with a wider voltage window, thermally stable as well as forming a protective layer on the surface of the anode, was essential for the next generation Li-ion battery system. The second reviewer was pleased that cell making and testing equipment was now available in the PI's laboratory as this would increase the relevance to DOE goals. Additionally the second reviewer said that without an electrochemical evaluation it was very difficult to see the relevance and suggested the voltammetry of the test electrolytes on platinum and glassy carbon would be a valuable initial screening technique that could be simply done would also increase the relevance of the work, particularly towards high voltage systems. The final reviewer commented that the project team was looking at new electrolytes that used a combination of new salts and also much higher concentrations than usual, and that this



work also involved development of ionic liquids for Li-ion batteries. This reviewer said success in this area could help modify and stabilize the interfacial properties of the electrodes, which could improve cycle life and lifetime of high energy batteries. In addition, some of this work could reduce electrolyte flammability and stability.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer affirmed that the basic approach was sound for seeking new electrolytes for lithium batteries. The ideas were novel and had a good chance of success in chemical terms. The reviewer observed that the difficulty would come in addressing such issues as validation and costs. The validation issue should have a broader focus as suggested under relevance. Electrolytes should be subjected to voltammetric tests after the conductivity/structure screening, followed by cell tests for successful candidates. In addition, the ideas of mixed ionic liquid (IL)-salt-solvent should be pursued aggressively as these solvents presented a truly novel approach to new electrolyte scenarios. In this vein, the viscosity of the electrolyte should be assessed as well as wetting properties toward electrodes evaluated to assure compatibility with electrode structures (a simple drop spreading test may be sufficient for wetting). This reviewer pointed out that the dianion approach seemed to be a difficult one with little payback. The closoborane dianions were carefully evaluated some years ago with no particular advantage shown. The simpler dianions generally have very low solubility in most aprotic solvents. The second reviewer indicated that the investigators have chosen electrolytes with chelated and - anions such as LiBOB and TFSI and solvents such as nitriles and lactones. This reviewer felt as though nitriles

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had shown good promise. The final reviewer expressed that this group was using a variety of experimental and modeling work to better characterize and understand the physics and interfacial chemistry of concentrated solutions. The early emphasis on acetonitrile as a solvent remained somewhat questionable as the reviewer did not believe this had much relevance to Li-ion batteries. However, the project team felt that this was a good model system that enabled it to hone its techniques for more recent work that was more relevant to EV applications. The reviewer remarked that the project's technical approach has been outstanding and the use of modeling in close collaboration with experimentalists has worked out extremely well.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer pointed out that the progress in the past year has been very good. The IL approach seemed very interesting. Some of the new anions looked promising as well. For continued progress in the coming year it was essential to activate electrochemical tests in the PI's laboratory, as mentioned above. The reviewer suggested that less expensive ILs should be considered. The second reviewer acknowledged that the synthesis of new materials had been developed and electrolytes with LTDI showed good potential for use as new electrolytes with high stability and good conductivity. The final reviewer asserted that this group had significantly advanced the state of the art in terms of understanding the molecular interactions in concentrated salt solutions, which had much broader implications beyond the battery world. This was difficult work, but, through the project team's close collaboration and meticulous data analysis, the project team had provided new insight into these poorly understood materials. Moreover, the researchers also found several cases where the literature interpretation of data was in fact wrong. This reviewer mentioned that while such concentrated solutions were very viscous, the high salt content could make up for this to some extent, and the researchers have studied these materials in their liquid state down to very low temperatures (-100°C). The PI showed an extremely impressive grasp of these complex materials, along with a gratifyingly high level of enthusiasm. The researchers had done a lot of work together and have been able to explain their results, something often found more valuable than the results themselves. The reviewer added that the project was moving from physical studies into cell testing.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer expressed the need for an increased level of collaboration, particularly in the electrochemical area. The BATT cell building should be activated as suggested by the PI as well as working with Dr. Whittingham and others such as Robert Kostecki. The reviewer suggested that by all means the project should continue the NMR collaborations as much as possible as this was a complementary technique to the Raman work. The second reviewer remarked that the project had reached out to strengthen its choice of path to new materials. O. Borodin in particular provided quantum mechanical calculations and molecular dynamic calculations to help direct the path for success. This reviewer added that Zhi-Bin from Wuhan supplied the LiFSI for use in ionic liquid solvents and V. Bataglia supplied cathodes for test cells. The final reviewer pointed out clear evidence of very close collaboration between NCSU and the modeling folks (including the University of Utah and Oleg Borodin at the United States Army). This reviewer added that the project was moving from physical studies into cell testing and so would need to leverage their linkage to the LBNL testing program.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

One reviewer expressed the need to expand the electrochemical testing with voltammetry on platinum and glassy carbon. Another reviewer commented that the characterization of the new electrolytes and search for new electrolytes would be continued. The reviewer stated that work would concentrate on ionic liquids as the solvents with the molecular calculations and ragman studies to understand the interaction of ionic liquids with the electrolytes. The final reviewer observed that in addition to adding to their existing physical studies (conductivity, viscosity, etc.), the project team had good plans to characterize the chemical nature of these materials for use in an actual battery – looking at chemical stability, corrosion, performance in actual cells. While the PI was well aware of the drawbacks of ionic liquids as practical electrolytes, the project team had identified some very promising approaches going forward.

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

All of the reviewers agreed that funding for this project was insufficient. The first reviewer suggested that if the voltammetry equipment was not available, then this should be added to the laboratory. The second reviewer remarked that, given the success of the project, a funding increase should be considered due to the more rapid progress on this important finding on new electrolytes and their potential. The final reviewer fully supported this work and believed that it was actually underfunded. This reviewer recognized that it was not at all clear that these electrolytes would make it to commercialization for EV batteries, but the reviewer felt that this PI was extremely well-placed to explore this space in a designed, scientific exploration, rather than the empirical approach that was so often see in this area. The final reviewer would very much like to see the PI's work continue and expand to see what the PI could come up with. Ionic liquids and the concentrated blends offered a whole new class of electrolytes that could have a major impact on future batteries. This reviewer asserted that these were the folks to explore that space and wanted them to be given the chance to run with their ideas and to see what the researchers could come up with.

Molecular dynamics simulation and AB-Intio studies of electrolytes and Electrolyte/Electrode Interfaces: Dmitry Bedrov (University of Utah) – es058

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

One reviewer commented that the electrolyte was an important contributor to performance, cost and safety, and that this program intended to improve the understanding at a fundamental level of the electrolyte and its interaction with surfaces. Another reviewer stated that molecular dynamic calculations were the best method to identify promising avenues and speed the development of new battery technology. This reviewer added that ab initio calculations provided insight into structure and properties essential for future progress. The same reviewer opined that the investigator was a valued resource and has shown the ability to assist others in their work while carrying out the investigator's own projects. The final reviewer noted that the project was looking at the chemistry and physics of high voltage electrolytes and electrode interfaces, using ab initio modeling techniques. Both aspects were critical if high energy that some of the new cathode materials promise to deliver is ever to be leveraged. This reviewer added that this work aimed at improving stability that could

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result in higher cycle life and a much longer calendar lifetime of high energy density batteries for EV applications.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer expressed that this was one of the most complex undertakings in the program and considerable work has gone into developing an approach which yielded results pertinent to the DOE program as well as suggestions for experiment to test the computed results and to lead to better electrolytes. The second reviewer stated that no one technique was capable of meeting all the requirements for identifying the most efficient direction for scientific investigations. This reviewer added that a combination of *ab initio* calculations, reactive molecular, dynamics simulations, as well as classical molecular dynamic simulations were employed. The third and final reviewer remarked that this work provided understanding on an atomic scale that experimentation simply could not provide. The final reviewer added that this group did excellent modeling studies and that the group also worked in close collaboration with experimentalists to deliver relevant insights. In this project, the project team was also looking at materials very relevant to new high energy density batteries, both from and electrolyte and electrode point of view. Often, one of the hardest things for such modelers to deal with was deciding exactly what to model. The final reviewer felt that this group remained very focused and relevant to the task at hand.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer explained that the oxidative stability of electrolytes was the key to high voltage operation. The results confirmed that many solvents may be oxidized through the solvated ions. This work should continue to develop as many examples of low energy pathways for oxidation as possible for as many solvents as possible to bring further understanding to the field. The first reviewer remarked that validation of the electrolyte simulations would be tested using Raman spectroscopic; results had given confidence to the simulations. This work should also be expanded to as many test cases as possible. The second reviewer noted several aspects of the project. The reviewer listed *ab initio* calculations on oxidative stability and decomposition pathways of electrolyte components: Molecular dynamic (MD) simulations of Li-ion transport through an SEI; MD calculations of bulk electrolyte and their interaction with electroactive surfaces; and *ab initio* calculations of nickel-manganese spinel particle surfaces. This reviewer also stated that much of the work had been in conjunction in support of other DOE projects. The final reviewer stated that the project's ability to show exactly how the presence of an anion such as BF_4^- could influence the stability of a solvent by acting as a bridge in oxidizing a solvent at much lower potentials than it would otherwise occur if a different, more stable salt were used. Thus, for the first time, the researchers are able to correctly predict the experimental oxidation potentials for a variety of solvent/salt combinations. Although there was some variability among experimental oxidation potentials (depending on the substrate, current density cut off and even the purity of the materials used), the project had presented a consistent approach that meshed experiment and theory very well. The reviewer added that more importantly, the project team explained exactly why some salts destabilized the solvent to oxidation. This was a very important issue to understand as there is a move towards higher voltage cathodes in order to improve battery energy density. The reviewer acknowledged that the team had shown which faces of the high voltage spinel LiNi_{0.5}Mn_{1.5}O₂ are less or more stable and provided insight on the electrolyte/electrode reactions at the interface. The project models showed the actual structure of the electrolyte layers adjacent to the electrode surface, which could vary considerably from that of the bulk electrolyte. These effects were hard to determine experimentally or to predict theoretically without this kind of modeling work, but yet the effects are key to really understanding the surfaces.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated that the collaborations with W. Henderson on Raman spectroscopy used to compare results from simulations had been especially productive. This reviewer added that other collaborations were important to maintain. The second reviewer stated that the project provided significant services to ANL, Arizona State, NC State, ARL, Rhode Island and Pennsylvania State University. Additionally, this reviewer acknowledged evidence of a really productive researcher. The final reviewer observed clear evidence of a very close collaboration between the modeling folks and various experimental groups, which in the reviewer's view was an essential element of all successful modeling initiatives.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer listed: study electrolyte oxidative reactions of NMC surfaces with electrolytes; study the composition of the electrolyte-electrode interface as a function of voltage; Li-ion transport through the SEI and SEI composition; continue collaborations with ARL, URI, Pennsylvania State University, etc. This reviewer also suggested investigating the role of sacrificial additives for the SEI. These were common to Li-ion electrolytes but were closely held as proprietary to electrolyte suppliers. The second reviewer commented that understanding these interfaces was going to be crucial in developing solutions that provided the increase in energy that these and other new cathodes could deliver while still maintaining (or improving) high cycle and calendar life. The second reviewer added that indeed, the main value of this and other modeling work was not predicting reality but in explaining reality to a depth that could not usually be attained by experimental studies alone. Everything about stability and lifetime revolved around localized interactions in and between the material phases and this group was well-positioned to really explain these interactions.

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

One reviewer felt that the funding was sufficient and did not provide further comment, while the other two reviewers affirmed the project funding as insufficient. The second reviewer asserted that while the investigator seemed to be overloaded with work,

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the PI's level of productivity was amazing. The final reviewer expressed full support of this work and believed it was actually underfunded. In particular, the final reviewer stated more studies should be done on different types of cathode/electrolyte interface reactions, including work on cathodes coated with stabilizing layers.

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

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer remarked that eventually a higher energy anode to replace graphite was essential. The anode material must have lower irreversibility (first cycle loss) than graphite, as well as a higher capacity, better efficiency, and longer cycle life. The second reviewer stated that silicon anodes were the most promising anodes for delivering a major boost in Li-ion energy density. This reviewer pointed out that the PI was trying to improve upon the researcher's previous excellent performance with silicon anodes for high energy density batteries. Some of this work also looked at low cost manufacturing and materials designs for S anodes. Thus, these designed materials had a decent chance of being manufacture-able.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer stated that the approach was to



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identify new nanostructured anode materials to replace graphite. It must have a lower first cycle loss, equal or better coulombic efficiency and a longer cycle life. A new thermoplastic binder with elasticity would likely be necessary as well. Initially, micro crystalline silicon would be studied as a possible candidate. The initial work would be directed at silicon in the micro and nano particle as well as amorphous forms. A new thermoplastic binder with elasticity would likely be necessary as well. The first reviewer remarked that initially microcrystalline silicon would be studied as a possible candidate. The studied as a possible candidate. The second reviewer asserted that the PI had explored a diverse and very interesting set of approaches to attain high anode capacity, good cycle life while also reducing the initial irreversible capacity loss than was a major concern with Si anodes. In particular, the PI had focused on designing material structures with the functionality that was needed in a methodical way, rather than empirical studies that was often seen in this area. This reviewer indicated that the PI had built on past expertise and was designing and building up interfaces to minimize the irreversible capacity losses that could be associated with having too thick of an amorphous layer of carbon present on the Si anode material. The same reviewer further added that the PI was pursuing several approaches simultaneously and this increased the chances of success to make this a more robust program.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer stated that initial work has identified a material with 800 mWh/g with 40 cycles demonstrated using surface control additives to control stability. The reviewer noted a Coulombic efficiency at 99.8% with an irreversible loss of 13.5% on the

first cycle using a surface control agent. Initial work on binders showed some improvement over PVDF materials. The second reviewer acknowledged that this work showed an excellent understanding of the surface chemistry and how the impacts on anode functionality, irreversible and reversible capacity, and cycle life occurred. This work showed two different approaches that had been very successful. One used a salt and polymer interface that led to a stable material with excellent cycle life although capacity was limited to 800-900 mAh/g (which is still far better than carbon, of course). One of the researchers' better results was an anode that delivered 1,200 mAh/g while being very efficient (high cycle life) and having an irreversible capacity loss of only 15%. While the latter figure was still somewhat high, it was less than half of that seen in previous work. Moreover, some of this could be balanced out by the irreversible capacity lost at the cathode and/or by adding lithium to the cell in other ways. One indication that the value of this work to the program was well recognized was that it was the first highlighted in the overview presentation given by Tien Duong (ES108, Slide 7). The second reviewer pointed out that the other approach used an ICA approach that could boost capacity to 2,000 mAh/g (about half of the theoretical value), but this material faded quite rapidly. It would be interesting to see the results of combining these approaches. The second reviewer felt that like many of the nanostructured approaches, manufacturing costs remained questionable. However, to address costs, the PI also had demonstrated good capacity with a low cost system based on using sugars as a binder. This reviewer stated that while cycle life was not yet there, this work was also worthwhile.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer observed collaboration with Ford, LBNL and the University of Pittsburgh. The second reviewer remarked that the presentation listed some important collaborators although it was not really clear how active the collaborators were in this program. The second reviewer also added that close collaboration would become more important as these materials migrated up the ladder and became candidates for full cell testing.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer suggested continued preparation of silicon anode materials with 1,200 mAh/g capacity; and identification of additives to control first cycle loss and new thermoplastic binders in coin and pouch cell configurations. The second reviewer remarked on two elements of a promising anode and stated that there was indeed a good chance that combining them would be successful in assuring good cycle life while enabling a reasonably high reversible capacity that would be a step improvement over conventional graphite anodes.

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

The reviewers were in disagreement. The first reviewer deemed the funding sufficient and provided no further discussion. The second reviewer felt funding was insufficient. The second reviewer expressed that the quality and the sheer amount of work done by this PI was very impressive and recommended an increase in funding for this PI.

Metal-Based, High-Capacity Li-ion Anodes: Stanley Whittingham (Binghampton University-SUNY) – es063

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that the anode performance was a limiting factor in Li-ion cell performance and noted that improved performance was essential. The second reviewer observed that this program was aimed at developing a tin-based anode for high energy density batteries. The reviewer remarked that this was important because, while not quite so attractive as silicon from a capacity viewpoint, it still offered a chance to significantly boost cell energy density while avoiding or at least alleviating the stability and safety issues researchers were running up against in trying to get silicon to work. As such, it represented an important area of research for the EV program.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer expressed that emphasis on low-cost tin and silicon materials should result on new high performance materials. This reviewer added that one or both may be successful. The second reviewer felt that



the basic premise was good - going for tin which, while not as energetic as silicon, was still potentially far better than carbon anodes. Moreover, tin promised to be more stable, less reactive and maybe safer than silicon. As such it represented an important area of research, especially if silicon could not be made to work. The second reviewer pointed out that almost everyone else was looking at silicon, but silicon was a somewhat risky approach, especially for EV applications where long calendar and cycle life were required. It actually may be more practical for consumer goods where such demands were less stringent (although safety was still absolutely critical). The second reviewer expressed that in a way, the work on tin should be viewed as insurance in case silicon does not prove successful. The second reviewer did not think that starting with Sony's Sn/Co/C matrix was really well thought out. This reviewer remarked that this technology obviously never went anywhere, most likely because it had a poor cycle life. The approach seemed rather empirical and the reviewer hoped for a more designed approach to developing a Sn anode.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer acknowledged that Dr. Whittingham had the knack to develop new technology that met or exceeded expectations once the program started. The second reviewer asserted that the group appeared to have identified a promising alloy for follow-up work. While capacity was about two times that of carbon, the higher potential of tin anodes (leading to a lower cell voltage) somewhat reduced the potential gain of these sin-based anodes in real cells. Nevertheless, these materials remained very interesting and should be followed up on.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions? The first reviewer noted work with PRIMET, LBNL, BNL and NYBEST. The second reviewer observed that the project team seemed to be working well both with material companies to make these nanomaterials and also with the DOE labs for cell testing (LBNL) and fundamental studies (BNL).

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer commented that the new work continued the atomization of the nano-Sn-Fe and Sn materials. The second reviewer stated that despite some reservations about the approach (cobalt), the team had identified some promising approaches that should be followed up on. The second reviewer observed that the PI was well able to follow up on their initial findings in collaboration with the partner labs.

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

One reviewer felt that the project could use more funding given the productivity and creative ability. The second reviewer found the funding sufficient and pointed out that the annual funding for this project was not large, but continuance at the same or slightly higher level seemed warranted by the promising findings to date.

Electrolytes - Advanced Electrolyte and Electrolyte Additives: Khalil Amine (Argonne National Laboratory) – es066

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that the use of additives to improve cycle life was well established in battery chemistry. The search for them had been largely random until now. This program hoped to bring some scientific method into the search for new additives. The second reviewer observed that the approach was to couple calculations and experiment to develop additives leading to longer cycle life as well as a long calendar life. Quantum mechanical models of the materials directed at understanding and prediction of the functional additives for the SEI layer on active materials as well as shuttles for over charge protection by limiting maximum cathode potential. The second reviewer mentioned that the identified materials would be synthesized and evaluated in cycling and calendar life situations. The final reviewer commented that the concept was to modify the electrolyte to deliberately form a stable protective coating (the SEI) on the surface of high energy density cathodes being developed for high energy density batteries. An approach like this was needed to ensure the cycle life and lifetime of these improved materials. The final reviewer observed that this work was aimed at



developing both new solvents and additives to fulfill this function.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer acknowledged that the authors were experts in the use of quantum chemistry to determine reduction potentials and reduction pathways. The approach was a good one, but it was not clear how each chemical additive would be characterized for inductive effect, steric effect, etc. of substituent groups. This reviewer stated that the experimental part would be enhanced by securing a certain level of statistical analysis for the evaluation of additives, repetition of experiments to lead to error bars, etc. This would give more confidence in results. The second reviewer commented that quantum mechanical models coupled with experiment were used to identify and develop additives to form a stable SEI layer on carbon and cathode materials as well as overcharge protection additives for longer, more reliable performance of Li-ion cells. The second reviewer commented on the project approach that it consisted of closely coupling theoretical and experimental results to better understand stability and decomposition pathways in order to guide the experimental program. The final reviewer observed that this project made extensive use of model calculations to predict material stability, oxidation potentials and degradation reactions at both the anode and the cathode. In particular, the work to better understand the electrode interface with the electrolyte and the reactions that could occur there could be very helpful in understanding this critical aspect of cell chemistry that governed cycle life and calendar life of the

cells. The project team was also using the calculations to determine the oxidation potential of possible overcharge shuttle compounds before doing the synthesis and lab work to evaluate such materials.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer stated that the results for various chemical types were very good as far as it goes. The reviewer suggested that it would be helpful to try to establish some general rules as a result of the calculations, however. The second reviewer stated that the modeling work seemed to provide tremendous insight. However, the success in transforming this insight into solutions was not yet there. This reviewer felt that some of the additives, such as TTT, may work out but a dramatic improvement in capacity retention was not supported by the data shown. The second reviewer stated that most of the differences seen in Slide 15 were really in the initial capacity that then carried on over to the subsequent cycles. Thus, capacity maintenance with 0.2% TTT did not seem to be markedly better than control. Also, the meltdown in cycle life with one percent TTT suggested that either it was not very good at enhancing stability and/or there was another cause for the abysmal performance of this lot, which then called into question the reliability of the entire experiment. The final reviewer noted that *ab initio* calculations were used to predict reduction potential, decomposition pathway and protective film formation with close co-ordination of the experimental and theoretical activities. The project team started with an analysis of the present reactions of ethylene carbonate component of the electrolyte to better understand the formation of the SEI layer on graphite materials. The reviewer stated that the project team included DBBB additive limits cell voltage to 3.9 volts and added that the team mentioned that this did not hinder cycling at least up to 200 cycles.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer felt that the more collaboration of quantum chemical researchers, the better. The second reviewer listed collaborations with O. Borodin (ARO), D. Bedrov (University of Utah) and K. Gering (INL). The final reviewer mentioned good collaboration between the modelers and ANL.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer reported the following: improved modeling based on results to understand the electrolyte decomposition pathways leading to SEI layer formation; combined theoretical and experimental studies to identify new redox shuttles; and simultaneous identification of SEI additives with superior performance. The second reviewer stated that the plans seemed acceptable, but would like to see more lab evaluation of some of these materials once the modeling data showed the project had promise. The second reviewer recommended pairing up with LBNL to test some of these new materials that looked promising.

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

All the reviewers recorded sufficient resources for this project. The first reviewer stated that resources were adequate to carry out the planned program. The second reviewer noted that funding for this project seemed about right. Another reviewer made no comment.

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

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that new electrolytes with better stability were required for the next generation Li-ion batteries. This work provided the basis for identifying new materials with long life potential, especially for high voltage (above 4.5 volts) cathode materials. The second reviewer observed that the concept was to modify the electrolyte to deliberately form a stable protective coating (the SEI) on the surface of high energy density cathodes being developed for high energy density batteries. Something like this was needed to ensure the cycle life and lifetime of these improved materials.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer acknowledged that the focus of project was to investigate $\text{LiPF}_4(\text{C}_2\text{O}_4)$ solute in carbonate and ester electrolytes along with potential for additives that could form a protective film on 5 volt cathode materials, develop understanding of film



formation on cathode materials, also known as the SEI film formation on anode materials, and employ computational methods to screen and identify interesting additives. The second reviewer stated that the basic approach was to modify the PF_6^- anion structure by replacing two fluoride anions with an oxalate group for their LiFOP salt. This had the desired effect of essentially blocking the disproportionation reaction whereby the conventional PF_6^- salt forms F^- and PF_5 . PF_5 produced with the conventional salt was reactive and could cause further degradation within the cell. With LiFOP, the anion could not form PF_5 . The second reviewer also noticed that the project team was also looking at some other common additives (FEC, VC, LiBOB) and using ESCA to study their impact on the electrode surfaces. The LiFOP work therefore seemed well designed. However, the approach to the other additives did in general seem rather empirical and the reviewer hoped for a more designed approach to address solubility and reactivity.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer affirmed that the initial results showed good promise for phosphate, spinel and one-third cathode materials. Developed synthesis procedure for $\text{LiPF}_4(\text{C}_2\text{O}_4)$ solute, understanding of first cycle loss for $\text{LiPF}_4(\text{C}_2\text{O}_4)$ electrolytes. Good low temperature cycling, formation of stable SEI on graphite, good performance with silicon anodes with stable SEI formation. The second reviewer expressed that the project had shown some interesting results for a variety of anodes and cathodes. In addition, the project team had shown good performance in a PC-based electrolyte that, while it generally had better low temperature and rate properties, typically exfoliated graphite electrodes and/or generally led to poor cycle life. The project's PC/LiFOP electrolytes did

perform better at low temperature, but the conventional LiPF_6/EC blends did much better in terms of high temperature stability (55°C storage). Thus, the LiFOP was only a partial solution. The second reviewer also stated that the other main approach had been the incorporation of a base to try and suppress Mn dissolution. This seemed to be also partially successful in that it reduced the Mn concentration in the electrolyte by half. The researchers have done some good ESCA work to try and explain the results. However, overall the results to date were only fair. The reviewer did not believe that the project's conclusions about Mn dissolution or electrolyte oxidation causing fade to be novel.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer acknowledged good interaction with others including Abraham at ANL, Smart at JPL, Battagla at LBL, as well as Garsuch at BASF and Puglia at Yardney Academics, Li in China, and Guduru at Brown. The second reviewer stated that the project had a lot of collaborators. This reviewer hoped to see input on which additives to develop in design based on modeling or mechanistic studies.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer commented that future work built on the results of the work to date. Optimize $\text{LiPF}_4(C_2O_4)$ electrolyte at high and low temperatures, develop understanding of film forming additives for high voltage cathode materials as well as novel/new electrolytes for high voltage cathode materials. The second reviewer commented that the plans seemed acceptable in that the project was working on addressing the right problems, but that it was far from clear how the researchers hoped to accomplish their goals. Therefore, the second reviewer was not very optimistic the project team would succeed.

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

Both reviewers agreed that funding resources were sufficient. The first reviewer stated that the resources were adequate for the present program. The second expressed that funding for this project had been rather meager, but mentioned that it was hard to recommend any increase without more evidence of a concrete design plan to come up with a better additive.

Bifunctional Electrolytes for Li-ion Batteries: Daniel Scherson (Case Western Reserve University) – es068

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer explained that the project was to develop the ability to include flame retardants in the flammable electrolytes used in Li-ion batteries. This reviewer expressed that this would remove a very serious problem of fires resulting from damage to the Liion battery (as happened in a recent Volt battery fire). The second reviewer emphasized that the concept was to make an electrolyte component do double duty, such as act as a fire retardant or overcharge protection. In this way, the electrolyte could provide functionality that otherwise would have to be done using a higher cost additive.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer described that the approach was to identify flame retardant ions for inclusion in the electrolyte of Li-ion cells used in electric vehicles as well as other electronic applications. Functionalized anions containing phosphorus and boron impart flame



retardant characteristics to compounds fit the application would be studied using *in situ* spectroscopic means to develop guidelines for identifying functional relationship to guide the study. The second reviewer commented that the basic approach seemed fine, trying to get P, N, B into the solvent structure. The second reviewer expressed some concern that the amount of an additive or co-solvent required to confer non-flammability was often quite high with other additives reported (often 20%). The triol borates looked to be interesting; although this reviewer was not sure they would be inexpensive.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer stated that FRION II had been identified as a good candidate for further study. Compounds such as the reaction product of Li[PHB((OCH₂)3P]O would be identified and produced in sufficient quantities to conform their activity. The second reviewer indicated that the project had shown some interesting results, but they were not very promising. This work involved a lot of synthesis work, which was typically quite slow. Having said that, the researchers really needed to pick up the pace of this work in the reviewer's opinion and get evaluation data that showed some sign of real progress.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer noted collaboration with Dayton University using their microscale combustion Calorimeter and Novolyte for coin cell evaluations of the new materials. Both were outside of the vehicle technologies program. The second reviewer described
that the synthesis work was by and large an independent project that had little need for a lot of collaboration. Now that the project had some materials, the researchers seemed to have lined up some collaborators to evaluate outside of the DOE program. It remained to be seen how responsive the project team could be without being funded. The second reviewer recommended that the researchers work with LBNL to evaluate some of their materials.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer described that the project would continue to fully characterize FRIONS, etc., to build a knowledge base for a new class of safety-enhancing materials and that the project would also synthesize LiPoBr materials and derivatives. The second reviewer explained that the plans to evaluate their materials seemed fine, although as discussed above this reviewer recommended that the researchers work with LBNL to evaluate some of their materials. The project team needed to focus and get more evaluation work done to move this project forward before the project's money ran out. Without good supporting data, this reviewer feared that this would be a dead end.

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

Both reviewers agreed that the funding resources for this project were sufficient. The first reviewer indicated that when the project has successfully identified compounds, that additional funding should follow to develop a family of new flame-retardant materials. The second reviewer reported that the current funding level was modest, which was appropriate. The researchers did need to show that the project really had something useful to justify renewal after 2013.

Polymers For Advanced Lithium Batteries: Nitash Balsara (Lawrence Berkeley National Laboratory) – es088

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer described the project as using a block copolymer with no liquid present to make possible a metallic lithium anode and a much higher energy density than with a graphite anode. The second reviewer stated that separators were a significant cost element of Li-ion batteries and new, higher performance, lower cost separators were essential for use in vehicle systems. The third and final reviewer explained that the researchers were exploring new polymers mainly to help prevent lithium dendrites in lithium metal cells, but also to assist in blocking the solubility of sulfur species in Li/S cells. Thus, this work was aimed at enabling lithium metal rechargeable cells which, in principle, could deliver even more energy than improved Li-ion cells and would be a boon to batteries for pure EV applications where range anxiety was an issue.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer suggested adding an alloy anode such



as silicon to this work. The specific capacity could then be almost as good as lithium, but there was a little likelihood that dendrite formation would occur, which limited the present symmetrical and full cell work. Because the silicon would be encased in a block copolymer, the formation of an SEI would be minimized and the fade in capacity with cycling may also be much better than with a liquid electrolyte. The first reviewer added that the work on microporous separators should be continued with more emphasis than in 2012. The second reviewer suggested developing blends of SES triblock co-polymers and PS homopolymers to obtain nanoporous separator materials. The third reviewer reported that one of the project's approaches appeared to be to line the pores of a separator material with a copolymer that include styrene groups – these should add rigidity to the structure that could help prevent mix penetration of penetration by dendrites in lithium metal cells, for example. However, there was no way any of the polymers were going to compete with a liquid electrolyte as far as conductivity was concerned and in typical separators, the micropores were still large enough that the final reviewer did not believe conduction could be enhanced through a lining of the pore. This reviewer indicated that the researchers were looking at using the block copolymer as a stand-alone electrolyte imbibed with an electrolyte, which looked more promising. The reviewer admitted that the researchers were unclear as to what exactly some of the samples in the presentation were, especially in terms of the liquids present, and added that the slides did not make this very clear either.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer felt that this program continued to develop new results which were cutting edge in battery research. The second reviewer stated that it developed SEO block co-polymer that resisted/prevented formation of lithium dendrites for use in rechargeable lithium metal cell systems. This reviewer felt SEO electrolytes had a significantly longer life than PEO electrolytes. The second reviewer added that Li/SEO/sulfur cells are constructed with good cycle life. The third and final reviewer highlighted that the results showed decent conductivity, but never better than uncoated separator. This reviewer did not agree that the results showed the polymers are helping conductivity. It seemed clear that the project team was simply blocking/constricting the pores and added tortuosity to the separator material. The research may have value for the strength properties, the reviewer added, but there was nothing to suggest that the project team was having anything than a physical effect of the physical and conductive properties of the separator. Unless the pores were almost completely blocked with a polymer, the reviewer saw little hope that the transport properties could even reflect the chemical nature of the polymers; it was just a question of strengthening the material while doing as little damage as possible to the materials' liquid electrolyte conductance. This reviewer suggested that the stronger separators did help delay but not fix lithium dendrite formation. This reviewer felt that there was some progress made, but asked whether this could not also be achieved with a stronger conventional separator such as a polyimide. Cycle life was still too low to be that interesting, but maybe acceptable in conjunction with other features. The final reviewer emphasized that the work with Li/S cells was much more interesting because this could be a much easier and potentially cheaper way to constrain the sulfur species in the cathode and realize both higher energy density and reduce the anode corrosion reactions in the cell caused by soluble polysulfides. This could enable low cost, high specific energy cells, although the energy density of the Li/S system was not that high (uses light materials for both anode and cathode).

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer noted binder team leader interactions with Dr. Kumta (Pittsburgh University), Dr. Hickner (Pennsylvania State University), Dr. Liu (LBNL), Dr. Vaughey (ANL), and Dr. Hexemer (LBNL), among others. The other reviewer commented that the researchers listed a lot of collaborators, although it was not clear to the reviewer what the team was actually doing.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer suggested that the use of alloy anode could advance the progress substantially. One can refer to the comments under "approach" for more details. The second reviewer recommended quantifying the effect of SEO morphology on cycle life. This reviewer emphasized that a new separator materials was badly needed. The third and final reviewer indicated that the plans to look at full cells were good. This reviewer encouraged the researchers to give high priority to looking into the sulfur confinement issue as this could be an enabler for much higher capacity cells with better cycling efficiency.

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

Two of the reviewers provided a response for sufficient resources, while only one provided comment. Another reviewer recorded excessive resources. The first reviewer stated that the resources were adequate for the present activity but should be increased for the development of a potential lithium metal-sulfur cell. The other reviewer indicated that candidly, \$700,000/year seemed a lot of money for this effort. Maybe focus a bit more and reduce the funding a little, suggested the reviewer.

Electrolytes - R&D for Advanced Lithium Batteries. Interfacial Behavior of Electrolytes: John Kerr (Lawrence Berkeley National Laboratory) – es089

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that the work was relevant to DOE objectives as the only real hope for a dendrite free lithium metal battery was through the use of single ion conductors, whether of the polymer type as studied here, or of the glassy or crystalline solid type as carried out in other studies. This approach may accomplish the use of thicker electrodes which the other types had great difficulty with. The second reviewer indicated that single ion conducting (SIC) electrolytes were being explored as alternates to the present liquid electrolytepolymer separator construction. The reviewer added that single ion conductors eliminated concentration polarization and resulted in higher voltage cell systems, and that this represented a significant departure from present constructions. A flat discharge yielded a constant delivery of energy compared to energy curves where the current must increase as the voltage declined to deliver a constant power. The third reviewer mentioned that lithium true ionomers offered an extremely promising avenue to solid state batteries with excellent safety and



performance characteristics. Lithium true ionomers also tended to be somewhat rigid which could help suppress lithium dendrites in lithium metal batteries that seemed to be the only type of battery that could deliver the kind of range the DOE desired for pure EV batteries.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer commented that the approach had developed some novel types of polymers which utilized polysulfone or polyether backbones with silicon-based side chains to carry the anion moiety. The conductivity of the polymers was adequate for the studies when enhanced by the use of solvents (no salt solutes) such as EC and EMC. It may be desirable to utilize other solvents such as PC or TMS (since sulfone groups are already incorporated) to enhance the polymer flow or solvents such as 2-methyl THF or Dioxolane which were found to be good for the figure of merit in rechargeable lithium. The first reviewer was concerned with the problem of making good contact with very fine crystallite materials such as LFP and that increasing the polymer fluidity may enhance this effect and lower the interfacial impedance within the cathode and possibly within the anode as well. The second reviewer stated that the study of the lithium interface was also called for since the interfacial impedance of this electrode (in a Li/Li cell) is observed to grow steadily with cycling using the SIC. The concern was that an SEI may be growing on the lithium surface which would increase the impedance steadily. The reviewer also recommended the use of determining the figure of merit for lithium. If this value was not high

enough, there would be serious problems in cycling an optimized system (with limited lithium present). The second reviewer mentioned that the Li/SIC-LiFePO₄ system was demonstrated and has charge -discharge curves that are flat as opposed to sloping in the normal liquid electrolyte systems. This essentially doubled the energy delivery by the battery system and would definitely be worth exploring in detail, suggested the reviewer. The third reviewer indicated that the downside of ionomers had always been relatively lower conductivity than liquid or polymer electrolytes and more especially very high interfacial impedance at the electrodes. The tremendous advantage of the ionomers was that the salt concentration did not change during charge and discharge. Thus, the research did not suffer from concentration polarization in the way that conventional electrolytes do. Moreover, polymer electrolytes that are not ionomers also fail during actual use because the concentration gradients that develop during charge and discharge also drastically changed, for the worse, the transport properties of the layers adjacent to one or both the electrodes. Previous developments had improved the transport properties of the ionomers to the point where this was no longer the limiting factor. This work was aimed squarely at the major problems with high interfacial impedance and interfacial instability. The third reviewer commented that the researchers had designed their materials and used fundamental measurements to characterize them and then followed up this work with actual cell cycling under high temperatures. This had involved some careful synthesis work and also meticulous materials characterization and cell testing.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer acknowledged that the project had made some major progress this year by showing high efficiency charging and discharging of a full Li/LFP cell utilizing SIC. The cycling was only carried out at 0.1C rates which are not sufficient for a practical cell. The data on capacity and impedance were not shown for this condition, so it was not clear what one might expect for higher rate cycling. The anodic stability of the electrolyte was good on platinum, but there were concerns about anode SEI formation on lithium metal. This reviewer highlighted that the tin oxide results were not very good for cycling, but this was not too surprising as a conversion reaction was needed to utilize the material and this may not be very reversible with the polymer electrolyte. Again, contact with the electrolyte was a potential problem for interfacial impedance. The second reviewer stated that the project has demonstrated a model system with SIC gel electrolyte of polysulfone TSFI-EC:EMC electrolyte. Cells have delivered several hundreds of charge-discharge cycles. The system was stable at 80°C and contained lo Lewis acid salts such as PF₆. Hydroxolated nanotubes gave improved performance. Cells with SnO₂ based anodes also performed well with constant efficiency output. The third reviewer stated that this group has shown tremendous progress and the reviewer expressed optimism that this approach could yield the kind of performance being looked for. The stability of these materials and their interfaces after extended cycling at very high temperatures (80°C) was exceptional. Their use of the imide anion, which seemed to have a general plasticizing benefit in polymer electrolytes, avoided the thermal instability experienced with electrolytes containing PF_6^- anions. The third reviewer added that the researchers have shown major advances in terms of avoiding dendrites for cycling Li/Li cells, attributed in part to the strength of the materials but also the transport properties of the ionomers. The same reviewer opined that the materials the researchers were developing may also prove useful as an electrode/binder matrix even if used with a liquid electrode as it may enable thicker electrodes while minimizing voltage drops due to concentration polarization in the electrode. The shape of the charge/discharge curves bore this out. Much of this work appeared to validate the theoretical predictions underpinning this project, added the reviewer.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer noted a very high level of collaboration with other institutions. It would be good to seek out any groups with background in rechargeable lithium metal work from pre-Li-ion days. The second reviewer indicated collaboration with Molecular Dynamics modeling with Grant Smith and Oleg Borodin at the University of Utah. This reviewer also acknowledged Marshal Smart at JPL. In addition, this reviewer mentioned that the DOE Fuel Cell Program and Applied Science program at LANL Polymer electrolytes had the potential to replace the present liquid electrolytes used in Li-ion batteries and fuel cells for new polymer electrolytes. The third reviewer indicated good collaboration, leveraging partners both within and outside this program.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer reported that the future work was solidly based. The reviewer would like to have the PI consider adding a very small amount of a fluoride containing salt such as LiPF_6 in order to help build a passivating SEI. If it was thin enough it was possible that charging could occur mainly through the film rather than on the film. This could minimize the efficiency loss due to fresh lithium surface reaction with solvent. The second reviewer explained that the characterization of cell performance and evaluation of new polymer backbones should broaden the scope of this discovery. Attaching anions to the conducting carbon backbone and characterizing the new materials at Pennsylvania State University and NIST gave important information on the scope of the technology. The third and final reviewer agreed with their plans to look at the chemistry of the SEI layers. This reviewer suggested some baselining at low temperatures of their best-bet constructions, even at low rates, just to scope out the issues there. The reviewer added that also, the researchers may want to consider whether *ab initio* modeling of the interfaces could help them in their development work.

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

All of the reviewers indicated sufficient resources for the project. The first reviewer suggested that if progress continued that a doubling of the effort was in order. The second reviewer acknowledged that this group was making great progress and funding should continue. If the researchers saw value in adding modeling work, then increase funding for that.

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Diagnostic Testing and Analysis Toward Understanding Aging Mechanisms and Related Path Dependence: Kevin Gering (Idaho National Laboratory) – es096

Reviewer Sample Size

This project was reviewed by five reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer commented that converting lab information into field data was valuable. In addition, the database management was valuable. The second reviewer stated that diagnostics facilitated the identification of mechanisms and challenges at the material, electrode, cell and battery pack level. Such studies were crucial and should be pursued in parallel with material, cell and pack development. In some instances, the diagnostics provided key information about widely recognized problems. In other instances, however, the diagnostics studies indicated potential problems/difficulties of which researchers may be unaware thus pointing to new research directions. The third reviewer indicated that the project should help educate DOE and BATT/ABR/etc. participants and inexperienced battery suppliers towards a greater understanding of real-world battery life challenges and requirements which may already be well-understood by significant electrified vehicle automotive OEMs and experienced automotive battery suppliers. This should



indirectly promote greater realism and efficiency in addressing DOE's petroleum displacement objectives in DOE-funded activity and advance the capability of less experienced battery suppliers in the automotive world and in other markets. The fourth reviewer noted that there was a need for diagnostic to access the life of the battery to estimate battery warranty costs. The final reviewer explained that lifetime and cycle life remained key unknowns with new battery designs for electric vehicles that were critically important both from a view of assessing commercial viability and likely warranty costs but also in terms of reducing the uncertainty/risk associated with bringing on new products. Reducing this uncertainty could give auto makers the confidence that the researchers needed to bring new technologies to the market much faster.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer mentioned that path-dependent studies were good. In addition, pressure effects on aging addressed a real problem. This reviewer criticized that there were no obviously new approaches compared to what others had done previously. The second reviewer described that the project's goal was to establish a Developmental & Applied Diagnostic Testing (DADT) platform. DADT would be used to support advanced prognostics modeling tools (described in presentation ES124), examine mechanisms for cell aging (both at the cell and pack levels), improve materials and create protocols to minimize aging processes. The work was intended to serve as a bridge between laboratory cell test conditions and PHEV field test conditions. The third reviewer stated that the focus on exploring and advancing capabilities to consider aging path dependence was excellent. The use of

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wide variety of Li-ion cell sources was excellent. Inclusion of string-level studies was also excellent. The fourth reviewer remarked that the approach included all the stress factors and analysis of cells to determine the failure mechanism. The final reviewer believed that the researchers had taken a very sound approach to this work both in terms of rigor and looking at the right variables, while also using good judgment in constraining the battery testing to reasonable rather than extreme conditions. Testing to extremes was nice to do when one had the cell performance far exceeding needs and/or one really needed 100% reliability under all conditions. At a later stage, extreme testing may be warranted, but for now testing should be restricted to the challenging but real life test conditions the project had chosen. This reviewer agreed with the collaboration with Hawaii in part because Hawaii had done years of studies on driving patterns and actual battery performance in cars. This complemented the designed experiments that this program was seeking to carry out in the lab. This reviewer also liked the use of incremental capacity to help understand what was going on inside these cells.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer noted that the modeling of lab results was critically important to take advantage of the experimental work. The reviewer detailed that the determining factors that control aging, and connecting thermal management with particle fracture were intriguing and that the simulation tool was nice. The second reviewer indicated that a large number of Sanyo Y' cells had been cycled under various conditions (i.e., temperature) and protocols (i.e., duty cycles). The data did not suggest that there was any evident path dependence to the capacity loss with different duty cycles. The effect of severe temperature variations on the capacity losses, however, was quite significant. The study related to pressure effects on pouch cells seemed inconclusive. The influence of thermal excursions on degradation was also examined using a simulation tool. A Battery Database Management System (BDMS) was also under development to facilitate the efficient and timely extraction of large and numerous datasets needed for diagnostics analysis. In addition to INL, perhaps this was of utility to OEMs and others. The work was interesting, but did not clearly point to any significant revelations that would suggest modifications to procedures or materials development for battery cells and packs. The third reviewer stated "good so far", and looked forward to further progress. The fourth reviewer indicated that the simplified models to include some of the stress factors e.g. temperature, SOC, charge and discharge power were not formalized. The fifth reviewer explained that this work obviously took some time to get results one could trust. The Sanyo Y cells had been cycling for just over a year and the results to date showed the strong impact of high and low temperature during actual cycling, less so during rest. Running the cells at high SOC was also undesirable, continued this reviewer. The same reviewer further noted that these findings were not particularly surprising, but acknowledged that this approach seemed to be working out. While the reviewer reported that the cells had generally lasted well (the reviewer believed they were intended for consumer goods, maybe power tools), the cells were not intended to cycle as long as needed for an EV program. Thus, opined this reviewer, the cells had already faded below 80% capacity in most cases. It was not yet clear to this reviewer how the predictions from these cells could be applied to a totally different chemistry and cell design using current or future batteries designed for EVs. This reviewer also noted that it did seem as though the researchers had enough degradation to mine and analyze the data more than what was presented in the talk. Presumably the analysis was ongoing.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer noted collaboration with ANL and Hawaii. The second reviewer mentioned collaboration with the Hawaii Natural Energy Institute (HNEI) at the University of Hawaii and Argonne National Laboratory. The final reviewer acknowledged good collaboration between Hawaii and NREL.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer stated that all would be valuable in improving how lab tests were interpreted. The second reviewer explained that the project was essentially a continuation of existing work. It could be expected that useful information would be obtained, but whether or not it would be demonstratively useful for cell/pack development remains unclear. The third reviewer observed that the future research may not provide better aging models than what has already been followed. The final reviewer suggested to mine the existing data in more detail than shown in the presentation (which may have been already completed). This reviewer felt that it

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would be good to set a goal for the amount of degradation one needed to see in the cells to make viable predictions. The better the cells were, the more testing one may need. This could be a guideline for setting how much data one would need to make an estimate of the actual lifetime. If all one cared about was performance after 10-15 years, maybe the project testing would not have to be increased as the cells got better; an estimate of how much extrapolation one was willing to accept from a single set of standard tests might then be a more apt guideline for testing.

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

The majority of the reviewers indicated that resources were sufficient while the remaining indicated they were excessive. The first reviewer stated that sufficient funds were available. The funding may even be somewhat high relative to the insight obtained. The second reviewer liked the work, but noted that the amount of funding did seem excessive for this work.

Overview and Progress of United States Advanced Battery Research (USABC) Activity: Kent Snyder (Ford Motor Company) – es097

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer started that the USABC served as an interface between the technical community and the U.S. car manufacturers. It funded research and development efforts to mutual benefit. The second reviewer mentioned that this project supported the overall DOE goal of partly replacing the conventional vehicles with hybrid (HEV or PHEV) or electric vehicles, both to minimize greenhouse gas emissions as well as the national dependence on petroleum resources. This ongoing project (USABC) was a collaborative effort among the U.S. auto manufacturers and various U.S. battery manufacturers and the national laboratories in jointly conducting advanced battery research and development with shared resources from DOE, OEM auto makers and developing partners. The objective of this consortium was to reduce the cost of the batteries via increased energy density in high-energy (PHEV and EV) systems, and reduced cost via lowering the total energy content in HEV systems. Successful implementation of this project would result in



widespread infusion of battery technologies in vehicular applications, which would in turn reduce the petroleum consumption, and pave the way towards petroleum replacement. The third reviewer stated that this was the primary government cooperative effort with the U.S. automotive industry to work on advanced automotive battery systems.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer reported that the project allowed the car companies to share in non-competitive technology development that benefits all, manufacturers, national laboratories, universities and consumers, in developing new technology. The second reviewer felt that the approach adopted here was feasible and duly addressed the technical barriers of the HEV, PHEV and EV systems by identifying appropriate technologies and initiating programs for technology development as well as technology assessment. The objectives (since FY 2011) were thus to initiate and manage new and follow-on programs targeting reduced cost via increased energy density and life in high-energy (PHEV and EV) systems, and reduced cost via lower total energy content in HEV system. Other objectives included formulation of requirement sets for electrolytes and 12V stop-start applications, and to revise the existing EV goals. The approach here was viable with a variety of appropriate battery technologies being advanced, and was well-integrated with the material development efforts under DOE. The final reviewer said that the approach seemed to be more reactive to trends in the marketplace rather than innovating and trying to push the envelope.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer commented that there was progress in co-operation in all aspects of the developing EV market area, workshops to address specific problem areas, and funding for RD&E where appropriate. The second reviewer observed that good progress had been achieved in initiating several technology development programs addressing the needs of lower cost and improved calendar life for batteries relevant to PHEVs and EVs, as well as high power batteries and capacitors for Low-Energy Energy Storage Systems (LEESS) for HEVs. Notable progress had been made in developing hardware, i.e., suitable prototype cells and modules from SAFT, A123 and LG Chemical, and the thermal management systems for the LG Chem. Some of these cells, packs and battery systems were being tested in the national laboratories for their life characteristics. Also, developmental work had been initiated on the advanced (shrink-resistant) separators, perceived as key component in improving the safety of Li-ion batteries. Finally, several new programs were going to be initiated in the next few months (of CY 2012) to fill the technology gaps for PHEVs and EVs. Furthermore, a few workshops were held to formulate the requirements of electrolyte, 12 V stop start requirements and revise EV goals.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer pointed out that the researchers had an excellent balance in collaborations in all activities, work groups, and etc. The second reviewer stated that there were several useful collaborations with various national laboratories, e.g., in the testing of prototype cells, packs and battery modules. It would be more helpful, if through USABC, the battery manufacturers could assist the national laboratories in the development of next generation materials, for example in the infusion/demonstration of these materials in prototype cells and in the scale up of materials. Currently, there was only component development in DOE laboratories, but not a system level development effort, to which USABC contractors could significantly contribute.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer noted developing standards for 12 volt stop-start needed to meet CAFE requirements. The second reviewer remarked that the plans for future research were commensurate with the project, as shown here, i.e., to: continue initiating technology development programs with various battery manufacturers; finalize 12V stop-start requirements for potential program initiations in 2013; finalize electrolyte requirements for potential program initiations in 2013; and revise EV goals and requirements towards potential new future programs. These new programs were intended to address the needs of EVs more appropriately in the context of battery capabilities.

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

All of the reviewers responded that there was a sufficient allocation of resources. The first reviewer stated that the project seemed adequate and well-spent. The second reviewer noted that the resources were adequate for the planned effort.

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Progress of DOE Materials, Manufacturing Process R&D, and ARRA Battery Manufacturing Grants: Chris Johnson (National Energy Technology Laboratory) – es098

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer referred to an overview of the DOE for Materials R&D and the ARRA program manufacturing grants, over the period of 2008 to 2011 and the materials which resulted from the ANL programs. The second reviewer felt that this project was very relevant to the mission of the Vehicle Technology (VT) program to develop more energy-efficient and environmentally friendly vehicular technologies, which resulted in significantly less petroleum consumption and greenhouse gas (GHG) emissions. This project supported those goals by proving grants for various materials and manufacturing processes as well as ARRA funding for developing battery manufacturing facilities within U.S., with the objective of accelerating transition to the next generation of hybrid vehicle transportation. Under three different initiatives [i.e., Materials and Manufacturing Technologies for High Energy Li-ion Batteries (2008); Electric Drive Vehicle Battery and Component Manufacturing Initiative (2009); and



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Develop Advanced Cells And Design Technology For Electric Drive Vehicle Batteries (2011)], several developmental efforts were set up to accelerate the PHEV battery technology, which would result in widespread infusion of battery technologies in vehicular applications, and thus reduced the petroleum consumption. The third reviewer remarked that high energy, high power battery design and development of a manufacturing base in the U.S. for these types of energy storage systems were critical and necessary tasks to allow increased electrification of automotive drive systems and can result in improvements in energy efficiency and reductions in CO_2 emissions.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer felt that the program has empowered companies to establish Li-ion battery manufacturing in the U.S. as well as help the supporting structure of cell components leading to battery pack production for electric vehicles. The second reviewer commented that the approach being adopted by NETL was two-fold, i.e., to institute several technology developmental projects, with approximately 50% cost share from the developers, on various components of Li-ion cells and assist in the setting up of manufacturing facilities within the U.S. for Li-ion batteries of various chemistries as well as capacitors, and the associated raw materials. Under the materials and manufacturing technologies initiative, four programs were started on topics ranging from anodes, internal shorts, overcharge-prevention additive and scalable manufacturing methods. Under the battery and component manufacturing initiative, programs were set up for developing advanced cell, battery packs and battery systems. Likewise, in the

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manufacturing initiative under ARRA, several manufacturing and recycling plants had been set up in U.S. This reviewer acknowledged that the approach being adopted here was feasible and efficient, especially with the cost-share from the contractors, and addresses the key technical barriers (e.g., manufacturability and technology gaps).

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer commented that the industry had started to produce cells, batteries and battery packs for electric transportation needs. The second reviewer indicated that the progress achieved in initiating several technology development programs, based on cost-share related to the materials and manufacturing of Li-ion cells, on different materials was encouraging. Good progress had been accomplished in many of these individual programs. Some of the successful programs under the first initiative were the 3M project on nano-Si-C composite anode and the BASF project on the NMC cathode materials. In the recent set of awards, several new technologies: Pennsylvania State University's Li-S with carbon composite cathodes; Amprius project on Si nanowires; SEEO's PEO-block copolymer electrolyte; cell developing efforts at Dow-Kokam and Johnson Control; and Denso's thermal management scheme looked promising. Finally, under the ARRA battery manufacturing grants, several manufacturing plants were set up in U.S. on different technologies, even beyond Li-ion batteries, which bode well for the U.S. EV manufacturing. Some of them had already demonstrated production capability and it looked quite promising that tangible products would emerge from this effort that could benefit PHEVs.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer observed a good selection of companies and co-operation between materials and cell producers. The second reviewer explained that there was not much of collaboration across these individual programs, understandably due to the fact there was substantial cost-share from the developing organizations, which needed to protect their IP.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer noted no new information on the ARRA Program. The second reviewer mentioned that future plans included supporting the research and development programs on materials and manufacturing processes as well as supporting the battery manufacturing facilities. The focus on multiple technologies, as was being done here, would mitigate the risk considerably.

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

The first reviewer stated that in some cases duplication has resulted in the ability to produce more batteries, cells and materials than the present market could absorb. The second reviewer expressed that the resources were adequate for the overall project and most of individual projects.

Electrolytes and Separators for High Voltage Li Ion Cells: Austen Angell (Arizona State University) – es100

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that new electrolytes are the key to higher voltage systems. The second reviewer noted that new electrolytes and separators were needed for 5 V Li-ion cells. The final reviewer observed that this work aimed at developing improved electrolytes with better stability to high potential spinel cathodes (based on the sulfones) and thus could be an enabler for higher energy density Li-ion batteries. In addition, some of the materials had very low vapor pressures that might also offer some safety advantages.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer expressed that this was a difficult area for search, but that the approach had been productive in the past and likely to continue to be productive. The second reviewer mentioned that problems of liquid sulfone electrolytes had led to a diversion into solid electrolyte single ion study. This needed to be continued at a greater level of effort. The third reviewer explained



that the approach was to look at modified sulfones to overcome or alleviate their high viscosities while still retaining good stability. The researchers had encountered issues with stability of the materials and had changed direction to look at single ion conductors.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer found that the most interesting materials were the semisolids and single ion conductors. The second reviewer noted that a new inorganic ionic liquid had been identified with pure Li+ conductor. The liquid range was 100-350°C with stability to over 6 V. This was very remarkable and needed to be pursued with vigor. The final reviewer acknowledged that their work with sulfones was progressing well from a materials viewpoint, but they ran into stability issues with the high voltage spinel cathode. The stability issues were not well understood in the reviewer's view – and asked what the reactions were and if it could be a solvent impurity effect. The reviewer continued to ask if the modelers listed (Borodin) could not assist in explaining this. Also, maybe the problem could be addressed though surface modification of the cathode. This reviewer expressed concern that the sulfones were abandoned prematurely. The new work looked interesting and should be pursued, although the high activation energy of the new membranes meant that its conductivity was only greater than that of a conventional solvent-based electrolyte at 60°C and above. At room temperature and below, the conductivity was worse than that of the liquid electrolytes, but still reasonable.

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Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer suggested collaboration with John Kerr of LBNL, especially in the area of single ion conductors. The second reviewer mentioned Borodin (Utah), Chen (LBNL), Lucht (Rhode Island) and Zhang (PNNL). The third reviewer did not see much insight that could be provided by the modelers. Also, discussions/working with John Kerr at Berkeley was encouraged as he also had made some very nice progress on single ion conductors. The reviewer suggested that maybe ANL or LBNL could help better diagnose the instability issues with the sulfones.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer mentioned that a solid single ion conductor had been identified with good conductivity. Further characterization may result in a new electrolyte system for Li-ion batteries. The second reviewer expressed that it was not quite clear where this work was going, but that this could end up being an enabler for either high voltage systems or even a solid state battery with all the advantages that would bring. Also the reviewer was not yet ready to give up on the sulfones; the basic problem with these materials needed to be nailed down more, maybe by ANL or LBNL.

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

All the reviewers agreed that the resources were sufficient. The first reviewer emphasized the project may need increased funding to fully develop the new electrolyte. The second reviewer stated that this PI had an exquisite understanding of such conventional and concentrated electrolytes and ionic liquids and that these were important areas of research for future high energy density batteries. As such, continuing this work was supported.

PHEV Battery Cost Assessment: Kevin Gallagher (Argonne National Laboratory) – es111

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer commented that costs were critical for the success of the shift away from gasoline to electric propulsion. The availability of a model to predict the costs of various battery compositions was essential in developing viable research and development programs. It is also essential when decisions are made to continue a given technology into commercialization. The second reviewer mentioned that this project was quite relevant to the overall DOE goal of partly replacing the conventional vehicles with hybrid or electric vehicles to minimize the national dependence on petroleum resources. The (high) cost of batteries for PHEVs is a serious issue and is determined by the characteristics of electrode materials, among other things. The overall objective was to develop cost assessments based on appropriate models, for predicting cost and performance characteristics for battery pack values from bench-scale results and for predicting methods and materials that enable the manufacturers to reach the cost goals. The objective was in support of overall goal of developing a PHEV40 with a price less than \$3,400, weight not exceeding 120 kg, and volume within 80 liters. These



studies would guide the manufacturer in addressing the cost barrier for Li-ion batteries. The third reviewer stated that ANL had developed critically needed analytical tools for battery storage system design and cost.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer mentioned that a cell/battery was designed based on power and energy requirements, specific chemistries with accompanying costs. A report had been issued that detailed the model and its utility. The cost of the BMS seemed low. The second reviewer described that the approach adopted here was based on designing a suitable battery based on power and energy requirements for PHEVs and the performance characteristics of a specific cell chemistry and the required manufacturing facility and thus obtained cost calculations for advanced Li-ion electrochemical couples (LMR-NMC, LNMO, Gr-Si composite), and to predict the required materials and processes to reach the cost goals. The approach was based on similar models developed at ANL in the past and utilized the likely productions costs for the OEM manufactures in 2020, with due consideration for the materials improvements and high volume production of modules based on pouch cells. Since both the design and cost were coupled here, this model quantitatively correlated the impact of underlying properties, such as cell chemistry, parallel cells, electrode thickness limits, power to energy ratio and etc., on the total battery pack cost. The approach appeared sound, but there were a couple of deficiencies here: there was no consideration for low temperature performance (as well as high temperature life), which varied considerably depending on chemistry, and all the chemistries were assumed to have similar life characteristics, which was a huge

challenge for some of the new chemistries (e.g., Li excess LLC and Si anode). The second reviewer stated that the project was well designed and integrated with other developments in materials, processes and cell designs.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer indicated that these model calculations were essential to guide tech research and development efforts effectively. Assistance to the EPA in their efforts to set rules for Li-ion batteries was critical in arriving as a realistic rule setting. The second reviewer acknowledged that reasonably good progress had been achieved in carrying out the cost analysis for the batteries for PHEV applications and the results were not unexpected. Specific accomplishments included: completed and published BatPaC v1.0 with documentation model and a detailed report, and the BatPaC v2.0 and documentation was in progress; implemented both liquid (v1.0) and air thermal management (v2.0) in the model as well as pack integration components; and performed cost uncertainty calculation (v2.0). Some of the useful, but expected, trends were estimated cost reductions from high voltage and high-energy systems, increased electrode thicknesses and large-format pouch cells. Though these numbers were generated based on the information from an unspecified battery manufacturer, further validation of these cost projections was required by comparing with similar cost models or real data. Surprisingly, the costs appeared low both the battery management and thermal management. One difficulty associated with this model was that it was largely based on ASI data. Instead, it would be a robust model, if it was based on the real-time performance data over range of temperatures and discharge rates and lifetimes from the manufacturer's prototype cells. The reviewer noted that a more direct collaboration with the manufacturers of one or two representative chemistries in terms of using their electrodes/cells data would add credibility to these analyses and to the conclusions from this study.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer felt that a good cross-section of people was essential in developing models of this kind. The second reviewer stated that there were no external collaborations here, and it was entirely ANL in-house effort. A more direct collaboration with the battery manufacturers would be greatly beneficial.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer mentioned that the project would release/distribute into the ABR format for public use. The second reviewer observed that the proposed future research was to complete and distribute BatPaC v2.0 to the public, which included an evaluation of new evaluating new electrochemical couples and a further refinement of model calculations & parameters. Further, this project would transition to the new ABR format to support its other projects, e.g., voltage fade project, development of electrochemical couples and ABR facilities (CFF, MERF, Post-Test).

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? All reviewers indicated that there were sufficient resources for the project. The first reviewer noted that the release of the second edition of BATPAC supported EPA rule making. The second reviewer stated that the resources were adequate for the planned effort.

High Voltage Electrolyte for Lithium Batteries: Zhengcheng Zhang (Argonne National Laboratory) – es113

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that using high voltage cathode was one of many methods to improve energy density of batteries used for electrified vehicles. However, conventional electrolytes easily decompose at high voltage and cause a degradation of the cell life and performance. Development of new high voltage electrolytes was one of the key areas to be investigated for viable cell technology with higher energy density. The second reviewer commented that new high voltage electrolytes were required for higher voltage, higher energy, and longer life Li-ion batteries that would be required for the successful commercialization of electric vehicles. Synthesis of fluorinated carbonates, ethers, sulfones is needed to identify stable solvents, and conduct DFT calculations to guide the work. The third reviewer stated that high voltage electrolytes were critical to the development of high voltage cathodes leading to the next generation of electrolyte and are perhaps one of the more significant barriers to improved performance. The fourth reviewer indicated that as explained in the presentation, higher voltage combined with high capacity provided for both higher energy and



higher power which are desirable for transportation applications. However, it was not clear whether this was a sensible thing to do since electrolyte stability at 4V was still a problem. In fact the presentation illustrated the problem by using LTO anodes to avoid the reactivity of the solvents at the anodes. Obtaining a voltage window of more than 4V may not be a sensible objective.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer explained the approach as finding the best candidates through theoretical calculations, electrochemical analyses and evaluation of their effect with full cells having high voltage cathodes. The second reviewer described that the project was directed at identifying and developing new electrolytes for Li-ion batteries, experimental screening of organic compounds for greater than 5V stability, current-voltage curves with lithium metal and lithium titanium oxide materials, that fluorinated sulfone, ethers, ethylene carbonates were explored as electrolyte solvents for a start, and that DFT calculations were used to predict stability. The third reviewer mentioned that the approach seemed reasonably well thought out and that the screening data seemed clear and logical. This reviewer stated that a good job was done of explaining the relevance of all of the characterization data and the techniques were chosen appropriately for the task. The fourth reviewer stated that the approach was okay as far as it goes. The use of fluorinated materials had obvious problems at the anode but those might be solved by using an appropriate SEI formation. The presenter gave no rationale for why the electrolytes oxidized so easily when the theory said that the potential stability was much higher. This implied that some other chemistry must be going on. There was no approach to this, stated the reviewer.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer noted the decent effect of fluorinated solvent for obtaining better life with high voltage cathode compared to the conventional solvents. However, it was recommended to run some more studies on its trade-off by carrying out a full evaluation including power and low temperature performance tests. Also, the reviewer added that the development of its cost model would be a good addition. The second reviewer observed that the fluorinated ethylene carbonate had excellent cycling, capacity retention compared 5V spinel. Fluorinated heterocyclics showed promise and could be cycled at comparatively higher temperatures (55°C). Improved cell capacity faded for graphite anodes. The third reviewer asked if the DFT differences were significant. The third reviewer noted that the connection between performance and an anode interaction was implied but not made completely clear. The reviewer added that more time could have been spent on this. Ultimately this work needed more fleshing out to understand its true potential. The fourth reviewer indicated that much data had been obtained that would be useful and these had been worthy accomplishments. However, the theoretical basis for the work was not deep and the premise of the project appeared to be shaky. Lastly, the reviewer concluded that an answer to the divergence between theory and experiment was needed.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer noted decent collaboration with modeling experts and electrolyte experts at the United States Army Research Laboratory. The reviewer added that the project was nicely partnered with a national laboratory, universities, and an electrolyte manufacturer. The second reviewer reported collaboration mainly with ANL for calculation of redox potentials of the new materials. Daikin Industries prepared new electrolyte materials. Collaboration was with ARL and Conoco Phillips, Saft and EnerDel in industry. The final reviewer expressed that more collaboration with other DOE-funded groups appeared to be in order. The project did not have enough funds to do everything but the collaborations, particularly on the fundamental side, needed to be improved.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer observed clear plans for the next steps, including further characterization of cells with the proposed chemistries. The second reviewer noted the continuing search for fluorinated electrolytes with superior stability and defining the performance of promising candidates. This reviewer also noticed that the project would address reducing first cycle loss using additives. The third reviewer mentioned that some more materials-focused studies on the basic electrolyte thermal stability could be employed to help understand fundamental stability of the materials before entering the complicated world of full cells interpretation. The final reviewer cautioned that future research was very vague. Collaboration with a BATT project, for example, might provide better foundations for the work.

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

The majority of the reviewers found the resources sufficient. The first reviewer stated that resources were of the correct magnitude. Another reviewer mentioned that the project was seriously underfunded to achieve what was desired, but that the objectives were best served through more extensive collaboration.

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Spherical Carbon Anodes Fabricated by Autogenic Reactions: Michael Thackeray (Argonne National Laboratory) – es114

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that the project may provide an for energy density increase opportunity via improved/new anode materials. The second reviewer indicated that the electrification was expected to reduce petroleum imports significantly. This project was aimed at improving electrodes used in Li-ion batteries. The third reviewer mentioned that the aim of this work was to further expand upon Argonne's spherical carbon particles (SCP) used for Li-ion anodes. The researchers were trying to retain the good cycle life characteristics of their SCP anodes while boosting the capacity up to match that of conventional graphitic anodes – currently the SCP had about two-thirds of graphite's capacity. As such, this program could lead to a Li-ion cell with good, although not necessarily better, energy density that also had improved cycle life and maybe calendar life. Applying those concepts to some other materials or using different coatings could also lead to a modest increase in capacity.

Question 2: What is your assessment of the approach to performing the work? To what degree



are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer noted that spherical carbon particles were clearly of great interest and this work was a very significant contribution in that respect. The second reviewer asked what the yield of autogenic synthesis was. There were several steps that were needed to make the final product. This reviewer then asked if this process was commercially viable. Graphite and other carbons currently used in LIB have a cost in the 20/kg range. The reviewer continued to ask if this process could achieve that target. Similarly, was the additional step of depositing SnO₂ onto small carbon particles was commercially viable? The final performance was similar to graphite. The reviewer questioned if the additional cost was acceptable. The second reviewer indicated that the approach in terms of conversion of carboneous materials into spherical carbon particles was sound. However, the entire motivation for their application to anodes was somewhat not clear – was it to get improved safety through spherical shapes. The final reviewer remarked that the materials the researchers were working with were certainly elegant and the synthesis seemed fairly simple and scalable. The premise is that the anodes would improve cycle life and, and when combined with a SnO₂ coating, would still deliver good capacity. The reviewer opined that this seemed somewhat empirical in that it was not clear how these coatings improved reversible capacity, but maybe that was just a reflection of the time constraints of these presentations.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

One reviewer stated that the overall progress was excellent, but noted that the understanding and demonstration of abuse tolerance improvement seemed limited and unclear. Another reviewer asked a series of questions such as: whether there was a plan to study packing properties on small carbon particles; whether packing density was affected by the small size of carbon particles; whether graphite particles used today were typically much larger than small particles developed in this work, and whether or not there would be an effect on the energy density of LIB cells using this new material. This reviewer reported that it would also be useful to understand how SEI layer formation was impacted by the choice of anode particles. Would there be a need to ore-optimize SEI layer formation for small particles developed in this work, asked the reviewer. This may be challenging for cell makers who have had experience with graphite. This reviewer criticized that the cycling results for MCMB shown on Slide 15 were strange. Typically, it was possible to get much better cycle-ability with MCMB anodes. The third reviewer reported that the spherical carbon materials had been produced using a simple autogenic combustion type reactor. However, the main motivation was to produce smooth spherical shapes for materials that could be used to smoothen the current distribution, thereby removing possibly lithium whiskers and the corresponding safety issues, and etc. Also, there was another major motivation to produce these spherical shaped carbon particles with Sn and Sb to produce composite anodes. The reviewer opined that both the method of making spherical carbon particles and the post-synthesis high temperature treatment for improving crystallinity were fine, but, the project was not clear on the advantage of using spherical shaped carbons for producing composite anodes, added the reviewer. The reviewer suggested looking at the reasons for preparing these spherical carbons. The fourth reviewer indicated that the uncoated SCP materials had rather low capacity compared to the standard graphite, but that the materials had very good cycle life. The reviewer added that heat treating the material to make it more graphitic reduced the first cycle capacity loss, but did not significantly boost capacity. The researchers obtained a significant increase in capacity by applying a very thin SnO_2 coating that boosted the capacity up to that of graphite. However, fading of this material was higher than that for the uncoated SCPs and even higher than that of conventional graphite anodes. The reviewer noted that the capacity after 15 cycles was actually deficient compared to the control graphite. Thus, at this stage the material was not very promising. The fourth reviewer acknowledged that the concept of applying the coatings to other materials and/or using different coatings could prove valuable. Because the coatings were typically thin, this reviewer did not expect that the coatings in themselves could greatly boost capacity above that of the native material. The reviewer added that it would have been nice to have seen a better understanding of how these coatings worked.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated that the collaboration with an industrial partner for high temperature post treatment was good. The second respondent was not sure that this project needed much collaboration.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer asked what the reasons were for making particles even smaller. The second reviewer mentioned that planned future work seemed excellent overall, but any plan for further abuse tolerance characterization was either not mentioned or was absent. The third reviewer felt that future work was not very motivating. It was not clear on why and how sub-micron sized carbon spheres could help in producing composite anodes. Also, it was not focused on how the researchers would obtain such sub-micron spheres. The fourth reviewer indicated that the project plans seemed good, although the reviewer called into question the desirability of going to even smaller particles from a packing and electrode fabrication point of view. The reviewer noted that it could provide useful for fundamental understanding, though. This reviewer agreed with the concept of applying the coatings to more conventional anodes that already have a high capacity. A better fundamental understanding on how the coatings work would seem to be in order as well. Issues with hard carbons not addressed in the presentation were the typically lower density of such materials (reducing energy density). If this was the case with these materials, it would be something that should be at least acknowledged, if not addressed. The reviewer suggested that, at some point, studies to explore low temperature, high rate and sensitivity to Mn from cathodes would be valuable.

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Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? All of the reviewers indicated sufficient resources for the project to achieve milestones. One reviewer mentioned that the resources and funding were fine and the project team was making decent progress.

Novel Composite Cathode Structures: Christopher Johnson (Argonne National Laboratory) – es115

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer felt that, in general, the development of new positive electrode materials was nicely aligned with the national policy to reduce petroleum dependence in energy. This reviewer acknowledged that seeking different synthetic routes for battery materials better suited for PHEV was believed to be a correct approach. The second reviewer noted that this project addressed the improvement of a key material for increasing Wh/L, which may decrease cost, and reduce dependence on petroleum. The third reviewer asserted that the project supported the overall objective. The cathode powders being investigated were critical to the overall objective of petroleum displacement. The fourth reviewer indicated that this project was okay for proof of concept only. It was not a low-cost process as listed and required in objectives.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? The first reviewer noted that an ion exchange was a



powerful approach to treat an electrochemical material in contact with electrolytes. In addition, the rate capability of such a material should be better due to the open structure obtained by exchanging larger ions with smaller ones. However, regardless of the bulk properties, its electrochemistry was often limited by the surface layers of particles that may form later with cycles. The cycle performance was yet to be tested. This reviewer added that ion exchange methods were hardly new and were routinely used by others including the MIT group as listed in the literature. The second reviewer expressed concern about the process cost for this route. This reviewer questioned as to how much cost it added, and whether the process could be changed to reduce this cost. This reviewer was also concerned about the density and average discharge voltage. Mn dissolution should be measured and optimized too, added the reviewer. The voltage stabilization looked good, and the concept of putting Na in the structure was clever, stated the expert. The third reviewer stated that the ion-exchange synthesis was interesting and could provide well-defined materials. At some point, if something interesting and important was found, probably another or a simplified synthetic method should be implemented for practical purposes, suggested the reviewer. At the moment it was hard to know how easy it would be to scale this process. The fourth reviewer remarked that the use of LiBr for ion exchange made the process cumbersome from an industrial scale point of view.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer mentioned that when the material was discharged to 2.0 V, it was speculated that a significant amount of Mn(III) was produced, unlike in the pristine material. Thus, an extra amount of Li-ion may be needed, since there was no clear evidence of Li-ion site changes during discharges. It was questionable if the same capacity could be obtained in a full-cell configuration. This reviewer felt that this had to be demonstrated. In addition to the extra cost and slow processing, treating with a calcined material with a solution involving ion exchanges, e.g., acid-washing or the current method by PI generally resulted in a low density material. PI perhaps wanted to examine the tap density in consideration of electrode processing later. The PI mentioned characterization of the material by XANES. This reviewer questioned if the team had a plan to conduct or already carried out *in situ* XAS and/or XRD at APS. No data was presented. It was expected that critical scientific information was contained in the first two cycles. The second reviewer indicated a good rate of progress. This reviewer wanted to see full cell data at different temperatures, and some insight into how the process could be controlled to make consistent materials. The third reviewer acknowledged that excellent capacities were reported with some of the cathode powders. It could be of interest if in future presentations the authors mentioned the tap density obtained with some of these powders. The stacking fault and edge defects observed with some of the powders were a nice accomplishment. The fourth reviewer noted some good TEM and cycling data. This reviewer would have liked to have seen high temperature discharge at high rates, and full cell data. This reviewer asked how the surface area and tap density compared to the traditional synthesis.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated that the project collaboration and coordination was well-organized for basic studies and asked if there were any industrial partners or scale-up plans. No expertise in synchrotron x-ray based characterization team was seen. The second reviewer found it unclear how the collaborators contributed. The third reviewer emphasized important partners in national laboratories and academia and an industrial partner in the latter stages would be important. The fourth reviewer expressed the need to collaborate with others rather than only internally at ANL.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer stated that the ANL internal team was not known for *in situ* APS-based characterization. Unlike BES programs, a cost aspect may be checked, particularly on material processing (ion exchanges, cobalt incorporation, etc.). The second reviewer indicated that good directions were planned, but that perhaps too many directions were given at once. This reviewer suggested focusing on small amounts of Co addition, and optimizing the process for cost and performance. The third reviewer stated that full cell testing should be important. At some point discussions about tap density should be incorporated; since that was an important variable with strong practical implications, added the reviewer. Electrode fabrication should be discussed at some point too. These powders may require a slightly different electrode preparation. DSC seemed to be important too, added the reviewer.

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

The majority of the reviewers indicated that resources were sufficient, while one reviewer noted excessive resources. The first reviewer stated that the ANL resources were the best in the world. The second reviewer remarked that at the moment, the resources seemed sufficient. However, if a new development came along that required special attention, additional resources may be required. High energy cathodes were a key driver for batteries designed for propulsion applications, added one of the reviewers.

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Overview of Computer-Aided Engineering of Batteries (CAEBAT) and Introduction to Multi-Scale, Multi-Dimensional (MSMD) Modeling of Li-ion Batteries: Ahmad Pesaran (National Renewable Energy Laboratory) – es117

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that yes, this main Computer-Aided Engineering of Batteries (CAEBAT) project was a central component of the computer-aided modeling program launched by VTP in 2010. Its main aim was to speed up the process of designing batteries for plug-in electric vehicles, which aimed to use electricity instead of petroleum as the fuel source, so this would support the objective of petroleum displacement. The second reviewer felt that if successful, it could really aid in the faster development of advanced propulsion batteries. The final reviewer observed that this project provided a set of quantitative tools to evaluate automotive battery designs and predict battery cell, module and pack performances.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?



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The first reviewer mentioned that the project appeared to have gotten off to a strong start, with portions of work delegated to subcontractors who were focused on modeling phenomena that occurred at different scales within batteries. The open architecture of the CAEBAT program enabled various modules to be added readily, and it should be easy for all parties to continue to refine their tools as the understanding of battery behavior grows. The relevant parameters were passed between modules that handled the physics occurring at different scales. Both prismatic and wound battery geometries were handled. It looked like the modules would add up to a very thorough approach. The second reviewer expressed that on paper, the project looked very well-organized, involving parties who brought in considerable expertise in their own fields, but the success of these activities would depend on the ease and relevance these packages brought to the battery developers. This reviewer was reminded of the TLVT work performed within the DOE program and was not sure if any battery developer actually used it. This reviewer felt that attention needed to be paid to the fact that these packages needed to be innovative, elegant, tractable and as user-friendly as the researchers could be so that the project could bring real benefit to the users.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer indicated that there were some resulting simulations that modeled the current density and temperature distribution in these batteries. The results appeared highly plausible, capturing subtleties that were specific to the cell geometries.

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The second reviewer stated that the progress appeared to be quite impressive. This reviewer inquired about the following: whether there was any modeling work on tab locations (prismatic) on the long side; whether there were now designs out there which considered such locations especially for EVs; and whether the temperature data matched those in real cells.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated that the NREL team was collaborating with industry and universities through its three subcontracts. Through the Open Source Architecture that CAEBAT uses, NREL was also collaborating with ORNL, another national laboratory. This reviewer felt that the amount of partnering was great. The second reviewer expressed real concern for this area. The reviewer observed that over the years, with respect to programs involving many participants, it had been a challenge to track and coordinate and often one runs the risk of losing momentum and focus. This reviewer felt that having separate PMs for the separate programs was a good idea.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer said that the chances of overcoming barriers were actually outstanding, but was not sure what the barriers were. The project seemed to be thought out well, with the open architecture for the system, so it seemed to be mostly a question of the contractor and subcontractors executing their respective portions of the CAEBAT model. Much of this appeared to be reuse of the computational techniques that had already been developed for battery behavior at different scales and converting it to fit within the CAEBAT modular architecture, so there was no major conceptual hurdle. Rather, it was a question of the researchers doing the necessary coding to make this conversion. The third reviewer asked how the final judgments would be made among the "three horses". The reviewer also asked: what criteria would be used to determine which consortium was successful; when the end of the program would be; who was going to market the software; whether it was open source; how the cost modeling got incorporated in the program; who the vendors are; and whether there were any plans to develop abuse-tolerance models.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? The reviewers all agreed that the resources were sufficient. One reviewer stated that the resources looked to be sufficient to pull together this large project.

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

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that there was relevance to the overall objective of petroleum replacement. The second reviewer stated that the advancement of CAE capability or speed for cell and/or pack modeling and simulation could support overall DOE objectives of petroleum displacement. Any significant focus on standardized battery CAE software did not support overall DOE objectives as monopolization of this industry could stifle both innovation and further advancement.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? One reviewer indicated that the program looks very focused.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

One reviewer was quite impressed with the progress



already made. The other reviewer felt that understandably, it may be too early in the project to elaborate on any significant technical accomplishments or progress.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer acknowledged that the data sharing among the participants seemed very encouraging. This had always been a big issue among the participants. The second reviewer observed that collaboration with JCS and A123 was good, but additional collaboration with other, more diverse battery developers would be even better.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer questioned whether abuse/cost life prediction and would be part of the package. The second reviewer noted that it generally looked good. This reviewer felt uncertain of the background on potential particular focus on electrolyte properties for future work. The same reviewer inquired about binder properties, separator properties, etc.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? The reviewers felt that the resources were sufficient. One reviewer stated that it could be more, though.

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

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer indicated that this project was a subcontracted portion of the CAEBAT program run by NREL, which indeed supported the DOE objectives of petroleum displacement through using computer modeling to accelerate the process of designing improved batteries for plug-in electric vehicles, which aimed to replace petroleum with electricity as fuel. The second reviewer mentioned that the battery cell design model was a useful tool to predict cell performance with many different battery material and design changes. With a robust cell design model, fewer experiments would be carried out and hence can save on time, effort, and cost by improving work efficiency with modeling tools. The third reviewer stated that the design and construction of the battery system, cells, BMS, temperature control, etc., were essential for the commercial success of electric vehicles.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?



The first reviewer expressed that GM was focusing on cell- and pack-level simulations for batteries, which made sense in light of its recent work designing the battery for the Chevrolet Volt. The group was applying known physics models to perform numerical calculations. The second reviewer pointed out that the models that were currently available and those that would be developed through this project were well defined and it clearly provided information on cell and pack level model strategies including details on cell level sub models. The third reviewer indicated that this presentation/discussion was a report on the design of the GM battery pack. The reviewer felt that it did not include detailed information, but was a good discussion of the design principles. Further, this reviewer expressed that GM's needs and LG Chemical's cell parameters served to start the technical design.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer criticized that this piece of the overall CAEBAT project seemed a little behind, but guessed that perhaps the researchers got a later start because choosing subcontractors was part of CAEBAT's work for the past year. Right now the status was that cell user requirements had been defined and completed, and a cell-level validation test was in progress. Pack-level simulation requirements had also been defined and completed, but much of that work remained to be done. The second reviewer explained that the input parameters from battery manufacturers were obtained for model development. Basic ECM and thermal models had been implemented, and cell level validation results were available from GM. Pack evaluation data was currently available for model development. The third reviewer pointed out that it was not possible to give a realistic opinion because of a

lack of details on cell parameters, electronic control algorithms for control, and cell construction. The cell design showed some end termination, which usually resulted in non-uniform current distribution in the same cell with resulting voltage loss appearing as heat inside the cell.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer stated that the GM team appeared to be collaborating well with the NREL lead team. The second reviewer acknowledged that it was not easy to get all kinds of physical properties of materials and design parameters from a cell manufacturer for accurate model development, but this team managed to get input parameters from the cell manufacturer. Lots of cell and pack data were available from GM and the modeling expertise including thermal analysis were provided by NREL, added the reviewer. The third reviewer noted monthly reviews but no details on the results of monthly discussions, implementation, change orders, etc.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer indicated that the GM team's plans for future research appeared to be heading in a very logical direction based on the overall scope of the proposed work. The second reviewer felt that the methods used for this project were clearly defined. This reviewer noted plans of validations for additional information for the model development. The third reviewer emphasized the typical engineering activities in generating a new cell/pack design. This reviewer felt that data was needed on reliability of the operations to make a good judgment.

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

All the reviewers indicated sufficient resources. The first reviewer observed that the resources to complete the work should be sufficient. Only about 11% of the funding from DOE had been spent so far, and the work achieved thus far seemed congruent to the expenditures. This piece of the CAEBAT project should be completed with the remaining money. The other reviewer noted there were adequate resources for a preliminary design but there was a need for validation to reach ISO requirements for automobiles.

U.S. DEPARTMENT OF ENERGY Renewable Energy

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

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer indicated that this project actually was a subcontracted portion of the overall CAEBAT project being done by NREL, which certainly had the aim of making the process of designing batteries for plug-in electric vehicles easier. Both projects were certainly targeting the displacement of petroleum. The second reviewer explained that the key issues associated with reducing the dependency on oil for transportation using batteries were the battery cost, life, and safety. Identifying and optimizing these attributes usually took years and was very expensive. The development of models that could fairly accurately predict how battery designs and materials used to develop these batteries could reduce both the development time and expense. This project went a long way toward developing and then providing an easy to use system that provided tools for both the battery developer and the end user (automotive companies) that would help identify systems to meet the goals of the user. This reviewer felt that the goals of this program to reduce cost, improve



safety, and improve performance of battery systems using modeling should be realized. The final reviewer commented that the project's goal was to develop an electrochemical/thermal (ECT) coupled model for large-format Li-ion batteries (cells and packs), as well as a materials database. This would then aid OEMs and cell/pack developers in accelerating the adoption of batteries for vehicle applications.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

The first reviewer observed that the EC Power model incorporated many known parameters from materials used in Li-ion batteries, and was modeling both performance and safety. EC Power was one of the subcontractors working with NREL on the CAEBAT project, so its contribution could be added to the overall project in a modular fashion like the others. The second reviewer asserted that the approach was excellent because of the early involvement of key partners such as a major U.S. based automobile manufacturer and a large U.S. based battery developer. Their early involvement allowed the program to go in a direction that would be most beneficial and useful and allowed for the validation of the model in real world conditions, by real world users and developers. This reviewer noted that the key concerns of both the battery supplier and the automotive industry could then be addressed in the model and consequently made it not only a useful tool, but a user friendly tool as well. The second reviewer pointed out that the technical approach also addressed the key elements associated with both life and safety – the overall addressing of the relationship of temperature and its impact on the system. The third reviewer reported that the ECT model would

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be developed for materials characterization, physicochemical models, advanced algorithms and experimental validation. This would be fused together by EC Power into the ECT3D model which would then predict performance, cycle life and safety. These predictions would be validated by the industrial partners (Ford, JCI). If successful, this would certainly be exceptionally useful, but the complexity of such a model casted doubt on the ability to do what had been suggested. Still, without the effort, it would not be known how close one could get to predictive capabilities for critical battery performance criteria.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer asserted that the project seemed to be making good progress in modeling the behavior at the scale it worked at. It was showing plausible results for the thermal, electric, and safety performance thus far. The second reviewer acknowledged that the program was only recently started and had made significant progress toward the stated goals. This reviewer described that initial reports included increases in the materials data base; delivery of ECT3D to NREL for simulations; and the start of safety modeling work, with work on the nail penetration safety test. Good correlation between the modeled data and experimental performance data had been observed. The third reviewer reported that the materials database was established. Material, thermodynamic and kinetic properties for common Li-ion battery materials were compiled for variable temperatures, compositions, and SOC. The reviewer asked how this was done and where this information originated from. The ECT model was created and safety simulations (nail penetration and shorting with metal particles) had been performed. This reviewer stated that preliminary validation was underway. Although the results were interesting, it was unclear what new insights they offered thus far. The reviewer continued to say that if the results helped up the validation, the model may be very useful, given the complexity of understanding safety challenges. The prediction of life and degradation mechanisms, however, was expected to be quite difficult.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer indicated that even within its subcontract, EC Power was collaborating closely with Ford, Johnson Controls, and Pennsylvania State University. The second reviewer described that the key strength of this program was related to the collaboration with other partners. These partners included both key representatives from industry and capable representatives from a university. This reviewer affirmed that the way the program assigned the tasks to the partners allowed each partner to concentrate on their strengths, while using input from the other partners. Additionally, the established real time feedback loop to the partners allowed for dynamic and rapid improvements in the model. A good deal of progress appeared to have been made in a relatively short period of time, and for minimal funds. The third reviewer observed that the project involved numerous partners from industry, academia and national laboratories.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer suggested that the projected future plans appeared to be an extension of the work conducted thus far, with pack behavior to be added to the cell behavior currently modeled. It was not clear how this would be approached or how it would synch up with the pack-level work to be done by the GM team (another subcontractor for the CAEBAT project). This reviewer would like to see more details about this, but generally the progress thus far seemed to be good, so building on the work thus far should not be a problem. The second reviewer indicated that safety was a key enabler for this technology and that the future plans included increased simulations related to safety concerns. The stated major involvement of the automotive manufacturer and the battery developer in determining what safety issues would be simulated was excellent as they were the primary players and end-users. Continued validation of the model was the key to making this a usable tool and that was a major future effort. This reviewer felt it would be good to get more definition on what the extensive cell and pack validation methods would be; and, what the refined user interfaces would be. The third reviewer discussed the continuation of current work with safety simulations. This reviewer observed plans to extend work to packs (from cells) and continued with validations. The reviewer added that the project began work linked to life-degradation modeling and the optimization of battery usage.

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

The reviewers felt that the resources were sufficient to achieve milestones. The first reviewer said that if the project was already 33% done on about 13% of the funding, the project was being run very well and questioned that maybe the portion reported done already was just based on the timeline. The reviewer pointed out that EC Power should not run out of money based on the project's current rate of spending. The project would have the wherewithal to add additional features. The second reviewer stated that the funds appeared to be sufficient for this program as it as a 50/50 cost-share program and the commercial partners were providing their shares. The work seemed to be progressing at a faster rate than anticipated, and additional work may be the result. The third reviewer said that the project seemed to have suitable resources.

Open Architecture Structure for CAEBAT: Sreekanth Pannala (Oak Ridge National Laboratory) – es121

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

The first reviewer stated that the project was very relevant and interesting. The second reviewer asserted that the project was very much related to petroleum displacement. In particular, the thermal management of a battery was critical for practical applications. The understanding of heat transfer within batteries was a practical and very important area of research and development. It had important safety implications. The final reviewer stated that this program was aimed at the standardization of models and bringing them together into a useful, consistent package. This would help bridge the gap between cell developers and systems engineers. Equally important, by bringing some discipline, clarity and consistency to the modeling efforts, the individual modeling efforts would work together much more easily. Thus, this work should improve the efficiency and utility of the other modeling teams.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?



The first reviewer observed there were solid thoughts behind the approaches. Of course, the goals were rather grand and it would be interesting to see how the three programs were incorporated into this architecture. This reviewer expressed that the success of this project would depend on how well the various programs could be built into this architecture and how well the final package could model the entire sequence of battery development. The second reviewer suggested that it could be of great interest if, at a later stage, this program developed some useful hints about the chemical or electrochemical behavior of the different cathode materials, its combination with anodes, etc. This was such a complex area that if the program could discover or put together a model that could simplify and explain certain battery issues -to battery people with limited theoretical knowledge- could end up being very useful. The third reviewer applauded the overarching approach taken to get a handle on and to coordinate the various modeling efforts. The reviewer continued to suggest that this project should bring the necessary level of discipline to the modeling work so that the individual modules could work together. Without this, one would end up with just a bunch of pieces and parts that do not connect to each other, rendering them virtually useless in predicting and understanding the overall system design. This reviewer appreciated the agnostic approach taken to enable them to incorporate modeling work from any of the three teams into this master model. This reviewer discouraged the reliance upon proprietary modules for two reasons: such a black-box could not be properly peer reviewed by other modeling experts in the program and without knowing the details of the module it may also not provide the desired degree of fundamental insight needed in such a model; and the master model was then held to be enslaved by the proprietary module - the provider could make changes without explaining them and/or could withdraw support completely

leaving the overall module orphaned and frozen in place. The third reviewer felt that the open architecture approach was interesting and would seem to provide a completely open system that was much preferred, especially vis-a-vis any systems relying on proprietary programs.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The first reviewer considered the presentation by the author as excellent. The progress was quite impressive in all facets of the work the team proposed. The reviewer was curious how customizable the package would be. The second reviewer stated that the program could end up being of great value if it managed to develop some trends among the different cathode materials, for example. This reviewer added that the program may be off a little in terms of absolute values, but at least the provided trends could be very useful. The same reviewer questioned whether the thermo-electrochemical-electrical model, for example, could be expanded to other cathode materials. The final reviewer observed that the project team had delivered a prototype open architecture program. Progress seemed good on the basic architecture, added the reviewer. It was hard to say from such a short review how the researchers were doing in incorporating the individual modules, which were still being developed, into the program.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The first reviewer observed good collaboration among the team members. The second reviewer noticed that there were strong interactions with other institutions. This reviewer highlighted the hope that at some point industrial battery companies would decide to engage a little more in this area of research and development. The reviewer indicated that it was nice to see three industrial partners already. The third reviewer noted that collaboration was absolutely critical here and the researchers need to excel here as this is what this project is all about. The researchers seemed to have the right linkages in place. This reviewer encouraged monthly meetings with each and every one of the modeling teams/PIs feeding into this program, not just NREL.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The first reviewer questioned how ORNL planned to incorporate proprietary information into its model architecture. The second reviewer indicated that increased portability to Windows could be of great value. Similarly, the incorporation of a cost model could have important practical implications. The third reviewer affirmed that the project team's plans going forward seemed very good and that this effort was supported.

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

The reviewers had mixed responses as to the resources. The first reviewer stated that it was hard to judge at this point if the resources were sufficient or not, but opined that resources probably were not if further interactions with additional institutions are not implemented. The second reviewer supported this effort, but found \$500,000/year to be a bit excessive for this activity. The overall work is important, but this reviewer did not believe it to be that hard or to require so much in the way of resources. It seemed to be mostly a coordination and computer/modeler interface design development and study.

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Energy Storage Monitoring System and *in situ* Impedance Measurement Modeling: Jon Christophersen (Idaho National Laboratory) – es122

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback was positive in this section. One reviewer stated that battery life estimation was related to the electrified vehicle warranty cost (for battery pack) and hence, an improved system for monitoring the battery state of health and predicting the battery life based on that could be a key tool for an electrified vehicle. A second reviewer offered that some of the concerns with an electric powered vehicle included the uncertainty of battery life and the predictability of battery performance during the life of the battery. Additionally, this reviewer opined that this program was intended to identify an *in* situ diagnostic and prognostic system that allows automotive OEMs to significantly reduce the anxiety that customers may have about these areas by establishing and setting meaningful warranty and replacement time periods, as well as the costs for the vehicle batteries. Furthermore, including a system that could accurately perform the stated diagnostic objectives would increase the confidence of both OEMs and customers in battery electric powertrains and allowed for



their increased acceptance. Finally, this reviewer stated that increased acceptance would reduce the use of and need for petroleum for vehicle transportation.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Comments received in this section were generally positive. The first reviewer indicated that the project identified the objectives and applications of the techniques for measuring AC impedance at a significantly lower cost than normal EIS equipment. Furthermore, the ESMS concept for this project was clearly defined. The second reviewer observed that much of the work done to establish battery SOH was based on no-load conditions, as it allowed for more controlled data selection. However, continued this reviewer, the most useful data was captured during real time usage. Additionally, the collection of the data during vehicle usage provided the opportunity for real time feedback to the vehicle system controller, and was less visible to the customer. This real time feedback could also be used to make real time vehicle system performance adjustments to provide for optimum vehicle performance, fuel economy, and battery life. This reviewer continued, saying that the program attempted to correlate battery SOH during real time usage to a no-load condition, using several systematic and logical steps. The approach first established the key metric that would be measured, how it would be measured, the conditions under which it would be measured, and then related the results. These results were then used to develop the hardware and software system that could become the basis for a system that could be incorporated into a vehicle or battery system for use in establishing the battery SOH.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments were generally positive in this section. The first reviewer remarked that the project had proven there was little difference between this cheaper technique and the expensive EIS technique. Also, the growth of impedance measured through this technique was shown to be correlated to the corresponding cycle life pulse resistance. A second reviewer expressed that the approach as mentioned was excellent and progress had been steady since the program began. Novel techniques to capture the key desired metric of wideband impedance were identified and a technique was downselected that met the most obvious need of short test duration. This reviewer observed that the decision was made to proceed with the HCSD method and that the prototype hardware and upgraded software had been completed. However, it was unclear whether this system would be able to test a full battery pack or if it was intended to check individual battery modules. It was also unclear why the FST system was not chosen instead of the HCSD system, as the FST (as stated) had the same test time and resolution, but required less computational capability. This reviewer concluded that these items should be made a bit clearer.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The comments received in this section were generally positive. The first reviewer observed good outcome through the collaboration with both hardware and software companies for the equipment, while a second reviewer stated that the collaborators selected for the start of the program were excellent. The second reviewer also opined that a battery industry partner, and later an automotive OEM, should have been included further along in the program. These additional collaborators could contribute to faster implementation and development. Finally, the reviewer added, this had the potential of becoming a valuable tool and was needed as more EVs and other electrified powertrains became available.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer feedback was generally positive in this section. One reviewer observed a clear plan for future work such as enhanced model development for better equipment accuracy and the investigation of bias voltage or transient effect for under-load measurement. A second reviewer offered that addressing the IMB limitations were key, especially when considering the cost of another system being added to the vehicle. Ideally, the system would be either implemented as part of the vehicle system controls or the battery control module. This was the reason, continued this reviewer, for the suggestion for a battery supplier partner and/or a vehicle manufacturer partner. The need for additional collaborative opportunities was expressed in the future work and the project should include a battery developer and automotive OEM.

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

The reviewers agreed that the project resources were sufficient. One reviewer added that the current list of collaborators appeared to support this level of funding, and if the work was to be moved forward in a timely manner, it required more involvement from industry partners who may be willing to provide matching funds. This reviewer emphasized that this may increase the resources needed.
Battery Ownership Modeling: Jeremy Neubauer (National Renewable Energy Laboratory) – es123

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback from reviewers in this section was generally positive. The first reviewer stated that the project provided useful perspectives on battery-electrified vehicle usage over life and relative ownership costs. A second reviewer remarked that the project was trying to provide models and predictions showing where BEV, etc., actually made economic sense for the end user. As such, it had the potential of providing insight on potential usage patterns and of becoming an important element guiding DOE programs and funding initiatives, incentive programs in various countries in the world, as well as being very useful to the auto companies. The third reviewer opined that the battery usage strategy by the OEMs for their customers may not be widely used because each customer may have their usage profile irrespective of what OEMs may recommend. The strategy may have some value if it was used to educate customers on the benefits available to them if they find it acceptable. This reviewer cautioned that new EV customers may interpret this strategy too difficult to follow to reduce TCO and may be discouraged to buy this type of new technology. Finally, a simpler approach



that told EV customers about the battery temperature, frequency of charging, aggressive driving may be good enough for the maximum life and TCO.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Comments in this section were somewhat positive. One reviewer acknowledged that the project was tackling an inherently difficult and complex area of predicting how various technologies were likely to affect real users without having good supporting models for battery degradation. This reviewer accepted being fine with doing the best one could do with what one had to work with, especially as the results could presumably be rerun when better source data and models became available. However, concern was expressed regarding known deficiencies in the source model and about the fact that some factors had not yet been included merely because good data did not exist. This reviewer suggested it better to guess or include what one felt was the best data, although this raised the perception of gaming the system. More importantly, this reviewer added, there were many assumptions built into the results shown (i.e., Slide 13 footnotes), which in and of itself were fine. The same reviewer acknowledged that the project team was trying to do a very complex task. However, this would seem to call out for a lot of sensitivity analyses to better define truly critical unknowns. Knowing the critical unknowns could give a much better appreciation of the validity and limitations of the modeling works and lead to a more useful package. Equally important was that the sensitivity analysis could then be used to target support work in the labs to improve the model's basis in those few critical areas. Thus, the reviewer concluded, leveraging this

work to actually direct some of the other lab work would be desirable, but that did not appear to be happening. A second reviewer stated that the total scope of assumptions included in many parts of the analysis was unclear, but at the same time it was understandable that it would probably be impossible to illustrate all of those in a twenty minute presentation. However, for example, some key assumption points which were unknown would include whether battery warranty costs were included in estimations; whether capital amortization costs were included in estimations; and whether variations in local fuel costs and/or electricity costs were included. The final reviewer recommended including battery swapping, fast charge, etc., which would determine TCO for the customers and businesses owning the batteries.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewer feedback was somewhat positive in this section. The first reviewer stated that findings and definitive statements regarding financial justification of electrified vehicle battery replacements, whether positive or negative, were helpful and could help direct focus of related DOE research and/or encourage further exploration of related DOE research. This reviewer added that the assumption of 100% state of charge (SOC) charging may be unrealistic from an actual OEM implementation perspective. A second reviewer acknowledged that the models incorporated a lot of key variables and that it was good that the project team looked at the distribution of driving patterns rather than just the average. The quality of the estimates seemed good, continued this reviewer, but it was only going to be as good as the assumptions made and cell models used. Thus, the reviewer stated, the conclusions had so many caveats that it was difficult to see how the project could be considered very solid at this stage. Hopefully, as things get narrowed, the confidence in the conclusions could improve to the point where this work becomes more valuable. This reviewer further clarified that a good rating was given not for the value of the conclusions, which was considered suspect, but because the project team seemed to have created a good model for answering some very difficult and important questions that just needed better inputs and a clearer assessment of sensitivity to the various assumptions.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The comments received in this section were generally positive. One reviewer acknowledged that the level of collaboration was useful and that, while greater collaboration with industry OEMs may be challenging, this would be of great benefit to this project's relevance. A second reviewer recommended that sensitivity work and the importance of the cell degradation model already identified by this work could really guide some of the other research activities in DOE's various programs, although that did not currently appear to be happening. Furthermore, collaboration and communication between this group and the rest of the program would be especially critical for this program to start delivering trustworthy conclusions. This reviewer offered that it would be preferable to use the modeling to direct the lab work, rather than the other way around.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer comments were generally positive in this section. The first reviewer affirmed that this was actually a noble effort, but needed more work to become truly useful and trustworthy. Further, that reviewer would like this work to at least identify the key unknowns, assumptions, and models needed to improve the model's reliability. Patience may be needed as some of the improvements in the key inputs may take some time to be developed by others. In the meantime, this reviewer would rather see this model used to identify those assumptions and areas that needed more resolution rather than presenting one model result. The reviewer also offered that, at this stage, this program might be best viewed as a source of guidance rather than providing absolute answers. A second reviewer recommended that future research combined the battery degradation model with the work of Dr. Kevin Gering (presented in ES124) because both needed the same model for future work.

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

The reviewers agreed that project resources were sufficient. One of the reviewers noted that while what the project team was getting seemed fine in terms of funding, funding to other groups may need to be boosted to fill in some of the key gaps in the knowledge needed to make this model as something one could trust and really start to leverage.

Developmental and Applied Diagnostic Testing: Kevin Gering (Idaho National Laboratory) – es124

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Overall feedback in this section was positive. One reviewer offered that warranty issues were a significant commitment without a firm basis for justification and decision making. Further, a framework for establishing the aging issues and life-modeling tools was badly needed and was being developed on this project. This reviewer indicated that there was very little published data on aging and concluded that reliable data and experimentation were essential to provide accurate information on the life expectancy of a battery system. The second reviewer stated that there was a need for diagnostics to assess battery life and estimate battery warrantee costs. A final reviewer acknowledged that the project should help educate DOE, inexperienced battery suppliers, as well as BATT, ABR, and related participants, towards a greater understanding of realworld battery life challenges and requirements, which may already be well-understood by significant electrified vehicle automotive OEMs and experienced automotive battery suppliers. This should indirectly promote greater realism and efficiency in addressing DOE's petroleum displacement objectives in a DOE-



funded activity and advance the capability of less experienced battery suppliers in the automotive world and in other markets.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Comments in this section were generally positive. The first reviewer observed that a model was constructed consisting of the thermodynamic, transport phenomena, as well as chemical and physical interactions, especially of the electrolyte with battery components, to serve as a standardized evaluation model for predicting battery life. This reviewer further noted that the mechanical aspects of loss of contact of the active materials and the mechanical stability of the electrode materials were elements of the model. A second reviewer identified the project's modeling approach as one built on evaluating the life based on the path dependence, including the seasonal temperature, duty cycle, SOC target and SOC window. Also, this reviewer pointed out that the drive profile and the rest variations were included. A third reviewer suggested that while the focus on exploring and advancing capabilities to consider aging path dependence was excellent, the focus on embedding capability in onboard device monitoring and control systems for automotive applications may not be realistic or appropriate.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments from reviewers were generally positive in this section. One reviewer opined that significant progress had been made in predicting battery life, causes for aging, and developing metrics for understanding aging processes. This reviewer added that these were chemistry specific and could be used to identify the best battery system for the application. Further, the changes in kinetic parameters and the thermodynamic framework of the reactions made it possible to quantify the behavior of electrochemical reactions in the battery and estimate the effect on capacity loss. A second reviewer observed that the results showed the capacity fade at various temperatures and SOC, but noted that the internal resistance change was not monitored. This reviewer suggested that the aging should include the capacity as well as power characteristics for estimation of life.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments in this section were generally positive. The first reviewer observed collaboration with the Hawaii Natural Energy Institute, ANL, and Dow Chemical that was directed at the path dependence and aging, testing and battery aging, and modeling of performance as well as some electrolyte development. This reviewer further offered the need for greater funding here. The second reviewer expressed that collaboration with a viable battery supplier having a significant global presence could be helpful and more useful in guiding some aspects of the aging path dependence studies.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Overall feedback in this section was positive. One reviewer stated that future work was directed at the temperature profiles for selected cities, variations in upper and lower boundaries, to assist in projecting battery life as a function of location. Furthermore, this project should be a good source for lifetime estimations. A second reviewer recommended that future work should include the life estimation of additional factors (e.g., target SOC and SOC window for cycling and calendar life). The final reviewer remarked that the plan for future work was generally excellent. This reviewer also cautioned that the plan for integration of Cell-Sage into actual ES monitoring and control systems may not be practical or of commercial interest to the automotive industry or other industries and therefore may be a poor use of the funds.

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

The reviewers disagreed regarding the adequacy of project resources. While two reviewers indicated that the resources were sufficient, another reviewer reported that the resources were insufficient. One of the reviewers noted it was useful work given the funding level and also offered support for greater funding and activity for this or generally similar efforts. Another reviewer expressed that the present level of funding was low for the nature of the work and the end payoff for the results. This reviewer affirmed that funding was incorrect for this project, and suggested that the USABC could also be included if not already involved.

Electric-Vehicle Battery Development: Herman Lopez (Envia) – es137

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback in this section was positive. The first reviewer asserted that high capacity cathodes were important to DOE goals. A second reviewer agreed that higher energy cathode materials were a key element in providing high energy rechargeable batteries for transportation applications. A third reviewer observed that this work was aimed at screening and developing high energy cells as well as integrating these materials into large pouch cells suitable for vehicle applications. Furthermore, this reviewer indicated that an important element of this work was aimed at fixing ANL's manganese-based high capacity cathode for high energy cells. This reviewer concluded that it also meshed well with the ARPA-E funded work on silicon anodes for even higher energy cells.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project welldesigned, feasible, and integrated with other efforts? Reviewer comments were generally positive in this section. One reviewer observed that the project team had looked at not only the individual components but also



their interaction all the way from single electrode to full, commercial-sized pouch cells. This reviewer noted a holistic approach that had led to fantastic results. A second reviewer reported that cells with manganese rich cathodes, silicon-carbon anodes and proprietary electrolyte were produced with 1 Ah and 20 Ah capacity, but stated that no details were provided on the composition of the anode, cathode, and electrolyte or on the cycle life. This reviewer cautioned that the long sloping voltage (4.5 volts - 2.0) of the cathode may present problems for the BMS control. The reviewer further added that the chemistry was said to be tunable for the application. The final reviewer commented that the approach was valid as far as the description goes. However, there was no mention of one of the important problems of the high manganese composite materials, which is the fade in voltage during cycling. The reviewer added that this did not show up in the capacity as much as attrition in the energy and impedance growth, and further recommended that these problems be addressed by the authors.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Feedback was generally positive in this section. The first reviewer commented that the worked presented here on the carbon anode/modified ANL cathode was outstanding, similar to the project team's outstanding work under an ARPA-E Grant on Si anodes. The project team had demonstrated an almost complete suppression of the voltage drop phenomenon, which was one of the key barriers to getting this material out of the lab and into actual products. Although this reviewer acknowledged that rate performance remained a barrier, the reviewer had not seen that anyone else even knew what the problem was, let alone had a clue

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on how to fix it. Using a sports analogy, this reviewer described that Envia seemed to have hit a home run while everyone else was in the batting cage warming up. The reviewer also pointed out that this design should be very interesting for consumer electronics batteries where the rate and power requirements were not so high. Equally impressive was the project team's ability to combine its advances into a finished package and its implementation with a Si-based anode under the ARPA-E program. The reviewer recognized that the project team had even developed a low temperature electrolyte for this cell system. The reviewer was emphatically impressed with the small outfit, and described it as innovative, focused and delivering the goods. This outfit was characterized as far and away the most impressive this reviewer had seen in this arena. The second reviewer reported construction of 20.5 Ah cells with 3.56 OCV that yielded 218 Wh/kg, with 1100 W/l. This reviewer further observed that no Wh/l was specified, but that a new electrolyte was developed with good performance down to -30°C. The reviewer added that cycling of the 20 Ah cell gave 600 cycles to 80% of original capacity, while 1 Ah cells gave 1000 cycles to 70% of original capacity somewhat dependent on electrolyte composition. This reviewer concluded that long term goals for cost were \$100/kWh. The final reviewer was only 4.35 volts. While the new electrolytes seemed to improve the cycling, the tests were now run at 45°C and the rate was C/1. This reviewer noted that upper and lower voltage limits were not given and the cell seemed to have an entirely different capacity. The reviewer expressed difficulty in knowing how to evaluate results under such different conditions with different cell types.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewer comments in this section were positive. The first reviewer described this as a corporate effort by a start-up, and by its very nature, one could not expect the project team to be very open. The reviewer offered that the project team has really worked well with ANL in extracting the knowledge, having not just acquired a license. Thus, within the framework of a for-profit organization, the collaboration has been excellent. The project team was also observed by this reviewer to be using outside labs to validate some of their results. A second reviewer reported that while no date was specified, cells would be delivered for testing to INL, SNL, and NREL.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer feedback was generally negative in this section. One reviewer observed little description of the proposed work and indicated that there was very general discussion of work on scale-up, cell testing, and material screening. The second reviewer suggested working on rate performance and checking out high temperature stability, then combining with Si anode work, but still keeping the carbon anode cell design going as a backup. A third reviewer commented that future work was not presented.

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

The reviewers disagreed on the adequacy of project resources. Two reviewers indicated that the resources were sufficient, while another reviewer stated that they were insufficient. The first reviewer opined that the project team should be given all the money it wanted so it could run with its inventions then license to everyone else. This reviewer added that the project team seemed able to make major advances in all areas of cell chemistry, all at the same time. A second reviewer offered that resources were adequate for the described work.

EV Battery Development: Nick Karditsas (Cobasys) – es138

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments in this section were positive. One reviewer explained that advanced lithium-ion chemistries with high energy densities were the horizon for PHEVs and EVs, aided by the rapid emergence of new cathode, anode, electrolyte, and electrolyte additive materials for interfacial stability or over charge protection, both within the DOE laboratories and elsewhere. In addition to the performance improvements with these materials, opined this reviewer that cost purity and manufacturability were also important factors in the overall cost, life, and feasibility of PHEV batteries. This reviewer stated that the objectives of this project were to develop scalable processes for manufacturing electrolyte materials, synthesize kilogram quantities of each material, and make them available for industrial evaluation in large-format cells. This reviewer offered that this program was a key missing link between the discovery of advanced battery materials, market evaluation of these materials, and high-volume manufacturing. This program would also reduce the risk associated with developing and maintaining a domestic, commercially viable, battery manufacturing capability. A second reviewer pointed out that the goals of this



work were to implement higher energy materials for improved Li-ion batteries (greater range) and also to lower costs, which was one of the main barriers to acceptance of this technology. The same reviewer reported that this work was focused on the battery pack design, thermal management issues, and on devising a complete product, and would form a framework for commercialization of new advances in materials and design.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Reviewer feedback was positive in this section. The first reviewer explained that the use of high energy cathode materials was key to low cost, high energy systems, and that the project team seemed to have a step-by-step approach to the work, which was good. The second reviewer remarked that the approach involved development of advanced cells, packs, and a thermally efficient pack module. This same reviewer reported that the cell development involved the study of two cathode materials (i.e., convectional NCM cathode and NCM with Li-rich layered-layered structure in coin cells, 18650 cells and full cells) while optimizing several design parameters such as particle size, porosity, composition of composite cathode, and surface coating for thermal stability, and optimization of cells design relative to safety devices and separator. The pack design involved the following, as described by the second reviewer: optimization of pack layout; use of advanced materials; simplifying, reducing or eliminating the cooling system; ease in assembly; and mass production. The reviewer stated that the approach looked comprehensive, well-designed, feasible, and was well aligned with the material development strategizes in ABR. A third reviewer opined that the approach seemed rather

timid. The reviewer continued that NCM with 40% nickel content in particular was, by some measurements, a lower Ni content than that already in use in some power tool cells that had been torn down and analyzed. Other than that, the basic approach seemed very thorough and well thought out.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Positive comments were generally received in this section. One reviewer observed excellent progress achieved thus far in all categories (i.e., materials for advanced cell designs, cell designs, and pack designs). Further, this reviewer listed significant accomplishments that included the following: demonstration of high specific energy of 165Wh/kg in large format cells with the conventional NCM cathode (150 mAh/g), satisfactory safety performance of cells with thermally stable electrolyte and separators, and enhanced life performance via surface treatment of cathode and anode materials; completion of the initial assessment of Liexcess LLC cathode, and demonstrated good cycle life with an improved electrolyte system and initiation of the development of large format cells (32Ah cell); evaluation of different separators and effects of different surface coatings/dopants on cathode; and verification of the benefits from new pack materials and component integration as well as assembly process improvement toward target attainment. A second reviewer noted that although results have shown a continually increasing power density with each change, the energy density had not increased significantly and was still far short of the goal. This same reviewer cautioned that while this may be acceptable for HEV, it was not so for PHEV, and recommended that the authors rethink the approach to improved energy density. The third reviewer recognized that the project team had tackled a whole range of cell material issues, looking to cathode surface treatments, electrolytes, and separators in a screening mode. The team had also made good use of computer aided design work and the final specific energy of the package was quite good. The same reviewer indicated that many of the goals had been met and that the project team was only a third of the way through this contract, the energy of the system should be increased to meet the specific energy and energy density goals. The reviewer pointed out that the project team had demonstrated good power ratios and improved cycle life, but low cost lightweight materials for pack construction were also important in bringing down the \$/kW and \$/kWh figures. The project team had devised the pack to minimize the effect of cold and hot ambient temperatures on performance and lifetime, although these remained challenges. The reviewer noted that this program was well positioned to take advantage of improvements made by other material suppliers. Furthermore, the same reviewer shared that costing information from this program on actual packs should also be valuable, although actual costs were not disclosed for obvious reasons.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Feedback in this section was positive. The first reviewer stated that there were several useful collaborations on-going and planning to be continued, as the material development and demonstration in improved cells and packs would continue. This reviewer added that there was little interaction with the DOE laboratories, which could be used to verify these promising results from Li-rich LLC cathode. Another reviewer acknowledged that this was a commercial company, so collaboration was typically never going to be as open as with an academic institution or a national lab. This reviewer observed that the project team had good relationships with its suppliers, such as BASF. This reviewer expressed the hope to see some validation work and safety studies in cooperation with Sandia as this work progressed.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer feedback in this section was generally positive. The first reviewer reported that future plans included the following: development of cell with 180 Wh/kg with NCM materials; optimization of cell design for mechanical and thermal configurations of module and pack; further improvement of Li-rich LLC by surface coating and doping for a better rate performance and with an advanced high voltage electrolyte; elimination or further reduction of the cooling system; and additional optimization and integration of components with low cost and less complexity. The same reviewer remarked that these plans were well integrated with the project objectives and addressed and mitigated the risks associated with the Li-rich LLC cathodes. The second reviewer stated that the project team's plans seemed acceptable, but indicated a desire to see that new anode materials such as those developed by Envia Systems were incorporated, if possible.

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

The reviewers agreed that the project resources were sufficient. One of the reviewers noted that the budget of \$1.5 million, including 51% of cost-share from the contractor, looked adequate and well justified, based on the progress accomplished and its significance. Another reviewer expressed that while this was a substantial award, Samsung should at least match this, presumably with in-kind staffing. This reviewer shared that pack design work was significantly more expensive than cell design as one needed at least prototype molding and/or tooling for many components to provide actual samples. Thus, the same reviewer commented that the funding level did not seem too bad, although this was basically subsidizing product development work that normally could be funded internally by such large corporations. However, the project team was at least returning results.

LEESS Battery Development: Kimberly McGrath (Maxwell) – es139

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback in this section was positive. The first reviewer observed good relevance. A second reviewer explained that one of the deterrent factors for the use of the current Li-ion batteries for HEVs was the cost, particularly if the high power batteries would have to be met by the battery. The same reviewer added that an alternate approach for this was to augment the Li-ion battery with a Low Energy Energy Storage System (LEESS), which would be an advanced electrochemical capacitor. The second reviewer remarked that the objectives of this project were to meet LEESS EOL power and energy requirements through the development of capacitor cells and develop a system that represented a significant advancement over commercially available capacitor technology, with enhanced low-temperature performance and amenability for low-cost manufacturing. Such an advanced capacitor-based energy storage system would accelerate the infusion of Li-ion batteries in HEVs and may also benefit PHEVs. The third reviewer pointed out that the program aimed to improve the performance and reduce the cost of capacitors, which aligned well with the DOE goal of reducing petroleum consumption. Low cost capacitors



could be married with a battery pack to create a hybrid energy storage system for vehicles. The hybrid energy storage system would allow the capacitor to respond to the vehicle's power demands and the battery to provide the energy. This could allow manufactured batteries to be optimized for energy storage since it would not need to respond to the instantaneous power demand. This could also potentially reduce the size of batteries installed in vehicles if the current buffer provided by the capacitor was able to increase the battery's life for a given use-profile. This reviewer noted that current battery discharge paradigms limited the depth of discharge to preserve battery life. If capacitors were able to increase battery life by minimizing the instantaneous power draw, then the battery's depth of discharge could be increased without reducing the overall life of the battery. This would allow for a smaller pack to be installed, which would be lighter and cheaper. Further, as expressed by the third reviewer, the higher power potential of a capacitor could enable a greater amount of braking energy to be harvested and used for tractive power, which would increase the HEV's overall system efficiency.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Overall, reviewer comments were positive in this section. One reviewer offered that the program seemed to be taking a holistic approach to developing a low energy, high power capacitive system focused on materials and system design to meet the performance, price and packaging targets. A second reviewer observed that the capacitor development involved identification of new cathode, anode, electrolyte, separator and suitable cell design architecture. Specifically, as indicated by this reviewer, the

approach included development of the following: electrolytes with a wide electrochemical window, good low-temperature conductivity and lifetime; improved cell via selection of anode and cathode electrode materials based on discrete structureproperty relationships and combinational screening; low-cost separator; and leveraging economical cell design to produce the lowest cost and smallest and/or lightest system. This reviewer further noted that the approach looked feasible, it addressed the technical barriers of power, life, and cost, and was well integrated with the ABR program objectives. The third reviewer recognized that it was a novel idea, although handling a lithiated anode did pose its own challenges. This reviewer inquired about the impact on manufacturing steps.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Feedback in this section was generally positive. The first reviewer asserted that progress accomplished thus far was quite encouraging and went on to list the following, significant accomplishments: identification of two best anodes with low ESR and superior cycle life, from the screening of 20 anode materials; initiation of combinatorial screening of multiple cathodes; optimization of electrode thickness, resulting in 10% reduction in cell weight; electrolytes with superior low temperature performance than baseline; identification of electrolyte additives for improved cycle life; low-cost separator from Porous Power Technologies; and development of system with thermal design. Additionally, this reviewer remarked that these results indicated that the progress demonstrated thus far was consistent with the project objectives and that all the scheduled milestones were met. The second reviewer observed that the program appeared to be progressing in a methodical manner. This reviewer added that Maxwell had identified the necessary development steps that needed to be taken with regard to the energy storage system components and was working through the development in terms of material vetting and selection. A final reviewer acknowledged that progress had been made on several fronts, but cautioned that key challenges remained, including weight, and above all, cost and volume gaps.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Positive comments were received in this section. One of the reviewers noted good collaboration among the competent organizations, and a second reviewer further specified that there were useful ongoing collaboration with URI and Porous Power Technologies, and new collaborations with the DOE laboratories, INL, NREL and SNL were being planned for life testing, thermal modeling and abuse testing, respectively. A final reviewer observed a strong collaborative relationship with the national laboratories, but suggested that the project team could potentially benefit from an OEM that could provide additional insight on the performance and cost targets that needed to be met for commercial adoption of the technology.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer feedback in this section was somewhat mixed. The first reviewer reported that future plans were aimed at the following: finalizing the anode and cathode electrode materials, electrolyte, and separator based on previous down-selection results; fabricating cells from a pilot line; fabricating and testing hybrid ultracapacitor cells in final system architecture; and completing a full manufacturing cost model for both the cell and the system. The same reviewer added that the planned work was effective in removing the batteries to the realization of capacitor technology for LEESS without any obvious risks. Another reviewer explained that the project team had attempted to mitigate risks by identifying multiple sources to supply key components so that the program's success did not hinge on a single supplier. This reviewer indicated that the remaining steps forward seemed like a methodical approach to achieving the program goals and further described that the project team was moving forward systematically to achieve the following: selecting the component materials from the identified pool of candidates meeting capacitor systems from the prototype cells; developing a cost model for systems and cells; and constructing and testing production cells and systems. This second reviewer noted that while the project team's overall approach was consistent with production releasing an automotive grade component, the presentation did not provide a discussion on the level of validation work that would be undertaken on qualifying the cell and system design before initiating the production phase. This would be key to ensuring that the product was robust prior to its being released for production. The final reviewer acknowledged that a good amount of progress

had been made on multiple fronts, but questioned whether a roadmap existed to close the large gap in volume requirement and cost.

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

The reviewers agreed that project resources were sufficient. One reviewer explained that the budget, with 50% cost share from Maxwell, looked reasonable for the hardware development being planned. Another reviewer indicated that the financial resources dedicated to the program seemed adequate for the development activities, but could be light for full production qualifying a component for high volume manufacture. However, the reviewer qualified this statement with the caveat that the reviewer had not been involved with a battery or capacitor development program in the past.

Novel High Performance Li-ion Cells: Keith Kepler (Farasis) – es140

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback in this section was positive. The first reviewer described that increasing the capacity of electrodes and employment of abundant transition metals for electrode were ways of reducing the cost of batteries. In addition, this reviewer noted that the project's approach was to bring a new cathode chemistry to increase battery energy density and reduce cost, which was a key parameter for formation of the electrified vehicle market. The second reviewer also observed that the project goal was to develop a cathode additive that could enhance practical, usable energy density for the cathode. Further, this reviewer stated, the precursors and process were intended to be low cost, thereby enhancing battery performance with a minimal cost impact. A third reviewer remarked that the project dealt with improving energy density, cost, and safety of energy storage systems.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Reviewer comments were generally positive in this



section. One reviewer expressed that the project was well thought out, and well executed. Further, opportunities arising from the execution of the program were identified, evaluated and accounted for, as part of future work. Another reviewer opined that the LFO/LVO cathode seemed interesting with higher energy density as compared to the LFP chemistry. However, this reviewer cautioned, it had low voltage (i.e., lower than LFP), which may be issue for electrified vehicles that did not employ an expensive voltage booster. It was suggested that additional cells with LFO/LVO cathode may be required to meet the vehicle-level voltage requirement. This same reviewer commented that while the general concept of employing LFO/LVO cathode material to boost energy density was very interesting, it would be better to compare its energy (i.e., specific energy) densities to those of NCMs or Ni-rich NCMs widely used for high energy cells for automotive applications. This reviewer reported that the approach included the recycled LFO electrodes and synthesis process, study of the reliability of the electrodes, and building cells with Vanadium oxide cathodes for testing and validation.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Overall, positive feedback in this section was received. The first reviewer observed significant progress in terms of modifying LFO materials for its stabilization and evaluation of its effect on the active cathode materials. This reviewer also reported that the evaluation of life and performance of cells with LFO was ongoing. The second reviewer noted that increasing the specific capacity was accomplished, the cathode was developed, and building cells had been started. The third reviewer asserted that the cathode

work was well done, but identified a missing project element, which was the comprehensive characterization of a test cathode formulation, in a baseline cell configuration, so that a broader performance assessment could be done.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Remarks in this section were mixed. One of the reviewers pointed out that collaboration was not made as clear in the slides as it should have been, whereas the collaborations were made clear in discussions during the poster presentation. Another reviewer recognized ANL as a good collaborator for this project, but recommended additional collaboration with other national laboratories to fully evaluate cell performance such as abuse tolerance evaluation with new chemistries.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer statements were mixed, overall, in this section. The first reviewer stated that future research solved the problem of electrode stability and anode to cathode capacity ratio. A second reviewer observed that the project had effectively reached completion although the presenter indicated a 90% completion point. The final reviewer recommended a more detailed plan for future work to include clarifying the tests (e.g., low temperature performance and life tests under accelerated test conditions) that would be included for full evaluation of cells with new cathode material.

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

The reviewers disagreed regarding the adequacy of the project resources. Two reviewers indicated that resources were sufficient, while another reported that resources were insufficient. One of the reviewers observed no issues, while another opined that support from ANL may be enough for material development, but collaboration with other national laboratories was recommended for full evaluation of cells with new chemistries.

3-D Nanofilm Asymmetric Ultracapacitor: Fraser Seymour (lonova) – es141

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer feedback in this section was positive. One of the reviewers indicated that the technology was targeted for use in mild hybrid or LEESS applications, as defined by USABC. This reviewer further noted that these had the potential for large-scale market penetration into automotive applications and similar applications exist in grid storage. The challenges facing ultracapacitive energy storage were correctly identified. Another reviewer observed that this program demonstrated the cost savings, improved performance, and life with a water-based, asymmetric ultracapacitor, which had a higher energy density compared to conventional symmetric ultracapacitors. Key features of the technology developed by this project were employment of 3D nano metal oxide film for positive electrode and bi-polar electrode design to increase energy density and reduce costs. A third reviewer relayed the need for lowcost supercapacitors with the performance and life capabilities in order to meet USABC goals.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?



Comments in this section were generally positive. The first reviewer acknowledged the correct alignment of project goals with the reported barriers, which were correctly defined with respect to USABC goals. A second reviewer observed that IONOVA seemed to pre-define the issues with the conventional ultracapacitors (both symmetric and asymmetric) and addressed the issues by using a novel electrode, less corrosive electrolyte, and efficient cell design. The final reviewer explained that using the aqueous electrolyte would increase the self-discharge and may limit the application for HEVs when there was a long storage (e.g. 30 days at the airport). This reviewer further stated that the bipolar electrode designs were very difficult to implement and the battery industry had tried the concept using Pb-Acid and NiMH batteries without significant success.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Overall, feedback in this section was generally negative. One reviewer indicated that developing high porosity, high surface area carbon was beneficial to supercapacitor development. Another reviewer noted energy density improvements but highlighted that the power density was not as well defined. This reviewer also pointed out that both cyclability and self-discharge performance results were concerning at this stage of the project. The same reviewer recognized that the presenter somewhat addressed these concerns, and further stated they were part of the future work. The final reviewer stated that highlights of technical accomplishments for each cell component were described in the poster presentation materials. However, initial performance of the

cell was mostly highlighted and no life related data was informed. Also, this reviewer reported that key performance for xEVs (e.g., low temperature power capability) was missing.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments received in this section were somewhat negative. The first reviewer observed decent coordination with electrolyte experts, bi-polar cell and full cell design companies to address the main issues, while another reviewer explained that key collaborators had not engaged significantly in this project, at this phase. It was clear to the second reviewer that the collaborators would provide valuable support once their phases of the project became active.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer feedback was generally negative in this section. One reviewer remarked that less work seemed to be done for cell design optimization and suggested a more detailed plan for cell design and evaluation of bi-polar electrode stacks. A second reviewer explained that future research should be represented in terms of work yet to be done, and gaps to project goals. Additionally, the description of future work was overly qualitative.

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

The reviewers disagreed regarding the adequacy of project resources. Two reviewers indicated that resources were sufficient, while another reported that resources were insufficient. One of the reviewers summarized that the program was over two years in duration, with less than five months left, and reported at 75% complete. Further, the perceived gaps between current status and goals appeared to be potentially greater than indicated. This reviewer also cautioned that extensive risk was associated with the systems integration aspect of the project.

Implantation, Activation, Characterization and Prevention/Mitigation of Internal Short Circuits in Lithium-Ion Cells: Suresh Sriramulu (TIAX) – es142

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer feedback was generally positive in this section. The first reviewer asserted the need for predicting and preventing the potential for thermal runaway in Li-ion batteries, and a second reviewer offered that understanding the internal short circuit mechanisms and finding test method representing the internal short was very critical for battery safety. This second reviewer further added that, without understanding the safety failure mechanisms, no safe device could be correctly designed to prevent severe safety issues. The same reviewer remarked that this type of investigation needed to be carried out for better understanding of internal short circuit mechanisms to enable the use of reliable and safe batteries in electrified vehicles. A final reviewer pointed out that it would have met the overall DOE objectives if a mechanism for mitigation and detection was included, and that this was described qualitatively in the poster discussion.

Question 2: What is your assessment of the approach to performing the work? To what degree



are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Comments received in this section were generally positive. One of the reviewers offered that the implantation of precursor of metal dendrite and monitoring from outside the cell had a lot of value for the automotive OEMs. Another reviewer observed that the approach was very logical, involving screening various metals causing internal shorts with time or number of cycles and finding the best candidate for this project. Further, this reviewer noted that validation tests with coin cells and commercially available larger cells (18650 cells) supported the mechanisms for the internal short circuit. A final reviewer explained that the test described herein was an extension of that developed by the Japan Battery Association. The specific objectives behind this particular study were not clear in the poster presentation. Finally, this reviewer offered that while the study demonstrated that the test was effective when contaminating the cathode, it did not clearly explain what form of cycling induced the short circuit, as opposed to standard formation and cycling.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewer statements in this section were mixed. One reviewer reported good findings and progress towards the project objectives. During discussion with the presenter, this reviewer learned of some information on a sensor that could detect the internal short circuit before an extreme thermal event occurred. More information on that sensor may be communicated in greater detail in the

future. A second reviewer remarked that progress was difficult to judge, as goals were not clearly defined. Although the project alluded to a method for the detection of soft shorts, this reviewer noted a lack of any science to support the claims. The third reviewer observed that the poster presentation did not disclose information regarding the mechanism of formation of internal short, monitoring for significant characteristics during the life of the cell, and thermal run-away. Thus, it was very difficult to assess the significance of monitoring to find the potential of internal thermal run-away.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Feedback from reviewers was generally negative in this section. The first reviewer noted that Tiax was working with their customers, while the second reviewer remarked that no information regarding project partners was available in the presentation slides. This second reviewer recommended that it would be good to team with a large cell manufacturer and apply the same test method to large format cells (at least 5 Ah cells), which would further validate the test method to find similar responses to smaller cells. The final reviewer observed that no appreciable collaboration was indicated apart from prior work.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments in this section were negative. One of the reviewers observed that future work was qualitatively described. Additionally, though detection methods were discussed, mitigation was beyond the scope of the proposed future work. A second reviewer remarked that no future work was clearly mentioned in the presentation slides, while a third reviewer asserted that there was no future research plan.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? The reviewers agreed that project resources were sufficient. One reviewer clarified that because milestones were not clearly defined, it was assumed that resources are sufficient.

Novel Anode Materials: Jack Vaughey (ANL) – es143

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback in this section was positive. The first reviewer explained that this work was aimed at developing new ways to study electrode structures using NMR and tomography to better understand how some of the new high energy anode materials actually change inside the battery during cycling. As such, it should bring a useful capability to the DOE's infrastructure in this area. Another reviewer observed that this study was arriving at a better understanding of how lithiated silicon interacted with its surroundings. Further, continued this reviewer, silicon materials are viewed as a potential replacement for graphite.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Overall, remarks in this section were positive. One of the reviewers stated that the approach seemed very good, and praised the use of NMR as it was not dependent on having an organized structure in the same way that diffraction studies are. This reviewer believed this to be especially important as the field goes more and more



into nanoparticles or particles with nanostructures where the materials are often found to be amorphous, which limited the amount of information that diffractions studies could provide. Another reviewer expressed that the ANL synchrotron would be used to better understand how silicon interacted with its surroundings in a battery environment, while nano- and micro-tomography synchrotron would be used to better understand the synthesis procedures and effects of cycling. This reviewer noted that studies included the interaction of silicon with the surroundings varying the loading, morphology, and thickness in the electrodeelectrolyte environment. The reviewer added that it should also be possible to study the electrode position of silicon, antimony, and tin in a similar manner. The same reviewer suggested identifying and assessing the role of electrolytes and irreversibility as well as SEI composition.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewer feedback was positive in this section. The first reviewer reported the following: silicon metal was deposited on copper foam with a 50 micron pore size; electrodes were cycled and gave over 250 cycles without significant fade; CuSix alloys were prepared and also cycled; tomography gave evidence of the effect of volume changes on cycling, as well as the depth of discharge; and *in situ* experiments were underway to provide information on Li+ diffusion in the electrode structure. The second reviewer described the project team as having devised and made some interesting structures, although their utility remained to be seen as it was still in the early days. Additionally, the project team had developed techniques and demonstrated some very good images of

certain key materials. In terms of capability, this reviewer found that the project team had made good progress on the tomography and was getting its NMR system up and running.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments in this section were generally positive. One of the reviewers commented that interactions included Cui at Stanford, Liu at LBNL, Whittingham at SUNY-Binghamton, and Thackeray at ANL, and a second reviewer observed that overall collaboration seemed good. The second reviewer had hoped that the project team could have worked with Clare Grey or her group at Stony Brook University for the NMR. The same reviewer suggested that Rex Gerald may also be worth consulting as he did some early work on *in situ* NMR of batteries at ANL and was still located there, though in a different division.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Feedback in this section was positive. The first reviewer reported that NMR would be employed to improve the understanding of the macrostructure of silicon electrodes and x-ray tomography for studying the internal structure and morphology relating to capacity fade. A second reviewer asserted that the plans seemed fine.

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

The reviewers agreed that project resources were sufficient. One reviewer indicated that the present funding level was adequate for the present program needs, but cautioned that additional funds may be needed in the future to speed development of commercial electrodes. Another reviewer opined that while the work was worth continuing, \$400,000 for 2012 was a little pricey.

Development of Si-based High Capacity Anodes: Ji-Guang (Jason) Zhang (Pacific Northwest National Laboratory) – es144

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer feedback was positive in this section. One reviewer explained that new anode materials for higher performance Li-ion batteries would significantly increase energy storage capability, while another remarked that this work was aimed at new ways to make high capacity silicon anodes for Li-ion batteries.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Overall, comments in this section were mixed. The first reviewer stated that the problems and potential solutions for the following were identified: mechanical instability of Si particles - nanostructured Si; electrical instability, loss of contact to active mass - conductive additives and coating; and electrochemical instability - new electrolyte and additives. Another reviewer indicated that two approaches were mainly used. This reviewer reported that the first was the core-shell approach with silicon inside a carbon shell, which seemed satisfactory, but was not especially novel. The other approach, continued this



reviewer, was based on using a very hard B_4C core and then coating Si on the outside. The reviewer did not see how this could help contain or handle the effect of Si expansion because the Si was fully exposed to the electrolyte. This reviewer opined that, in a sense, the B_4C seemed to act as voluminous, wasteful current collector. Additionally, because the B_4C comprised about half of the anode coating, adding this inert material cut capacity in half, with no real advantage observed from the second reviewer. The same reviewer expressed difficulty in seeing why one would expect this to work and concluded that some of the work seemed rather empirical (e.g., slides purporting to understand the additive effect described work that just evaluated the materials and did little or nothing to understand how it worked or did not work).

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Feedback from reviewers in this section was mixed. One of the reviewers reported the ratio of Si/Core/Graphite for optimum performance had been established. This reviewer also observed an electrode with 822 mAh/g capacity retention of 94% after 100 cycles with reasonable rate dependency had been achieved. Further, addition of FEC additive improved cycle life. The second reviewer acknowledged that the work on Si with large pores showed an advantage, but cycle life was still far too poor to be of interest. In addition, this reviewer noted that the Si in carbon framework studies showed decent stability and capacity, although not any more than many other approaches by other groups. The same reviewer also described the manufacture method as reasonable, and that even the data for the B_4C electrodes looked decent. However, the reviewer was unconvinced of the project team

explanation regarding why this worked at all. The PI indicated that the hardness of the balls compressed the Si and retained it in place, but the electrode structure was essentially open on one face, which led this reviewer to query why the Si could not just expand and squeeze out material in that direction.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewer comments in this section were mixed. The first reviewer recognized Princeton and Vorbeck for grapheme, Rhode Island for electrolyte additive, Vesta for porous Si, and North Dakota State for Si nanowires. Another reviewer did not get a feel for this in the time available, and though many partners were listed, this reviewer was unsure whether this work needed a lot of collaboration in the early stages.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Remarks in this section were mixed. One reviewer acknowledged an acceptable, proposed work plan. The plan, as reported by this reviewer, involved improving cycling performance of rigid skeleton concept, carbon layer, and porosity, etc., as well as characterizing full cell performance. This reviewer also noted the inclusion of a SEI layer study and additives. The second reviewer saw no evidence that the PI had a plan to really understand the project team's electrode materials, especially those with the B_4C core particles. The entire project seemed very empirical. This reviewer questioned that such work would lead to a significant advancement in the understanding of these materials, and without such understanding, progress or value returned to the program was doubtful. In another area, shared this reviewer, other PIs in the program were already working on additives and electrolytes to improve Si cycling stability. The reviewer inquired whether the project team could tap into them rather than trying to do this on its own.

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

The reviewers agreed that project resources were sufficient. One reviewer opined that resources seemed reasonable for the work plan, while another saw little reason to expect the project team to significantly advance the state of the art in this area.

ENERGY **Renewable Energy** Atomic Layer Deposition for Stabilization of Amorphous Silicon Anodes: Anne Dillon

Energy Efficiency &

(National Renewable Energy Laboratory) – es145

Reviewer Sample Size

U.S. DEPARTMENT OF

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer comments in this section were positive. The first reviewer explained that the focus of this project was on using atomic layer deposition (ALD) to make very thin stabilizing coatings on both anodes (i.e., Si, Natural Graphite - NG) and cathodes (i.e., LiCoO₂ - LCO) to improve cycle life and reduce the irreversible capacity loss. As such, this reviewer further added that these approaches promised to significantly enhance the useful capacity and especially the cycle life and calendar life of new high energy density batteries. Another reviewer reported that the project was directed at developing inexpensive processes for silicon-based electrodes, including HWCVD and ALD, as well as developing a better understanding of the process parameters.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project welldesigned, feasible, and integrated with other efforts? Feedback in this section was generally positive. The



project team, as indicated by the first reviewer, had shown a novel and excellent series of approaches to stabilizing the Si surface. The ALD coatings were thin so that it should minimize any adverse impact of the coatings on the rate performance of the materials. The reviewer stated that the project team was making full use of a variety of spectroscopic methods to really study and understand the materials interface and combining that with some good cell builds, electrochemistry, and impedance studies of symmetric cells to help clarify which electrode was responsible for what phenomenon. This reviewer also praised the fact that the project team was looking at non-vacuum methods that would be necessary to scale up such an approach. A second reviewer observed that the major problems of volume change, mechanical degradation on cycling, as well as developing a simple solution using ALD coatings on a nanoscale Si particle, were all addressed.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewer statements in this section were positive, overall. The first reviewer explained that scale -up of HWCVD revealed that the substrate temperature played an important role in preparing suitable electrode materials. This reviewer further offered that the formation of crystalline silicon was identified with Raman study and must be avoided for long cycle life. The same reviewer observed that Si/Cu electrodes stabilized by ALD of Al_2O_3 with excellent coulombic capacity. The particles became amorphous after the first cycle and gave stable cycling capacity. The reviewer also remarked that the coating seemed to improve the mechanical stability of the anodes. The second reviewer was very favorably impressed by the amount of work and progress shown

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by this team, which had made the materials and structures it was targeting and shown that the ALD coatings did indeed offer significant advantages in terms of boosting the cycle life. Moreover, this was true on all three electrodes studied. This had shown that the method had a very wide range of applicability and the project team had basically proven the premise upon which this proposal was based. The project team, continued this reviewer, had made a Si/C anode that needed no binder and had a high Si content (70:30 Si:C). The uncoated thick core shell Si electrode did have a high fade rate, but it started with a very high capacity (2,600 mAh/g). Applying the 3ALD coatings maintained the high capacity while yielding a dramatic increase in cycle life. While still fading, this was one of the most promising results this reviewer had seen with Si. The thick core shell Si electrode did have a high fade rate, but it started with a very high capacity (2,600 mAh/g). The reviewer expressed interest in seeing how this material benefited from ALD protection, and further noted the possibility that the project team could deliver extremely high capacity and good cycle life. This second reviewer also observed that the project team's work was also getting at some of the anode/cathode interactions in real cells that were often overlooked by groups doing fundamental studies such as these. This reviewer emphasized that the project team was using a good combination of electrochemical characterization paired with detailed surface studies. The rate studies showed that ALD coatings were thin enough to at least handle moderate discharge rates. While this may yet be an issue for EV/HEV applications, it seemed to be fine for more modest discharge rates, such as those used in consumer devices or envisioned for some grid applications. The same reviewer opined that ALD was too slow to be commercially viable, with the possible exception of high end batteries (e.g., microbatteries, where the cost and scale are less of an issue). Thus, the separate work by Tenant (in presentation ES162) under a new ABR award was very important to build on the excellent work that this group had done. The reviewer concluded that while the carbon nanotubes (CNT) work with NMC cathodes was also interesting, the commercial feasibility of CNT remained a concern.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments presented in this section were positive. One of the reviewers listed collaborations, which include SUNY Binghamton, General Motors, LBNL, University of Texas, and SSRL. Another indicated that the project team was very well connected to other laboratories, industry, and SUNY. Moreover, continued this reviewer, the project team was actually using these connections to move the project forward.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Feedback was positive in this section. The first reviewer opined that the volume expansion problem may be easier to solve than the first cycle loss in preparation of Si electrode structures. In addition, this reviewer reported that work on the core shell process and alternates would be undertaken to lower the costs. A second reviewer observed good plans and offered no further suggestions since per that reviewer, this group is doing excellent work already and beating its deadlines. This reviewer expressed enthusiasm in watching the project team continue its progress, and appreciated the emphasis on moving from a vacuum-based ALD process to an e-beam method that could be used at atmospheric pressure.

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

The reviewers agreed that project resources were sufficient. One of the reviewers offered that resources appeared adequate and the researchers had demonstrated a high level of creativity and ingenuity in developing the Si-Cu processing. Another noted that funding for this project is quite high, but reflected the varied work involved. This reviewer added that it was really too much to take in on a single poster. The level of effort observed by this reviewer was impressive and fully justified the funding level. The same reviewer concluded that the team was working very well on multiple fronts to deliver value back to the program.

New Layered Nanolaminates for Use in Lithium Battery Anodes: Yury Gogotsi (Drexel University) – es146

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer feedback in this section was positive. One reviewer communicated that there was a strong need to develop anodes with higher capacity than graphite, and suggested that layered ternary carbides and nitrides may prove to be the best replacement for graphite anodes because they have a higher capacity, less expansion, longer cycle life, and lower cost than silicon materials. This reviewer further stated that layered ternary carbides and nitrides and nitrides known as MAX phases offered higher capacity than graphite and lower expansion, longer cycle life, and lower cost than silicon nanoparticles. Another reviewer reported that this work was aimed at exploring new, high capacity anodes based on MAX materials such as Ti_3AlC_2 .

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Comments were somewhat positive in this section. The first reviewer reported the following: *ab initio* calculations to guide the selection of MAX materials and



to reduce particle size for long cycle life; modify surface structure (e.g., exfoliation) to increase lithium uptake; establish a family of MAX phase materials with superior performance; and develop an exfoliation process to increase surface area. The second reviewer explained that the project team evaluated a number of MAX materials and found that the materials did not work well, but then redirected the team's work upon discovering that exquisite exfoliated layers could be formed. The project team stated that it used modeling to guide this work, although the reviewer found there was little in the poster showing this.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Overall, reviewer statements were positive in this section. One of the reviewers observed the identification of MAX materials and process development for HF treatment and sonification to separate sheets of active materials. This person further stated that resistivity of sheets was comparable to graphite and it was hydrophilic in nature. The same reviewer concluded that materials had essentially constant capacity for 100 cycles or more and capacities ranging from approximately 100 mAh/g to 250 mAh/g. A second reviewer remarked that the MAX materials, by and large, did not work out. However, the removal of Al by HF etching of the MAX layers produced well-characterized MXenes layers that could be separated out through sonification and had interesting properties. The lithiation/delithiation peaks were quite high, similar to that for lithium titanate spinel (LTO). However, this meant a substantially lower cell voltage and associated loss in energy and power unless compensated for in other ways. The reviewer explained that LTO actually had high power despite the lower cell voltage, but the energy loss remained a big problem. The

second reviewer opined that Ti_2C and similar materials looked to be an interesting class of anodes from a scientific point of view. The project team had done good work and answered the question as to what these materials could do. Unfortunately, the materials seemed to have three basic problems that the reviewer identified as unattractive for future development: high potential that led to a low cell operating voltage; low capacity; and high aspect ratio particles (e.g., exfoliated materials) typically do not pack well and are, therefore, volumetrically inefficient. The first two characteristics in particular would seem especially hard to overcome, although the PI felt that the capacity could be increased with additional work. In closing, this reviewer pointed out that the synthesis of these materials with HF etching did not look cheap.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments in this section were mixed. One reviewer acknowledged P. Simon at Paul Savatier University in France and L. Hultman at Linkoping University in Sweden, while the second reviewer had not developed a feel for this the level of collaboration in the limited time available. The second reviewer observed that the modeling work was not highlighted in the presentation.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Statements from reviewers were mixed in this section. The first reviewer stated the following: evaluate different Xenes as anodes in cells; develop processes to reduce first cycle loss; and study effect of carbon additives for conductivity. Another reviewer stated that the materials seemed to have three basic problems that made them unattractive for future development: high potential that led to a low cell operating voltage; high aspect ratio particles (e.g., exfoliated materials) typically do not pack well and were, therefore, volumetrically inefficient; and low capacity. This reviewer suggested to first focus on materials that have, or at least might have, a lower potential so that cell voltage would be higher. Otherwise, the reviewer observed, no chance that this would compete with graphite. It would even have a problem versus LTO because the commenter believed it was more expensive to make. Thus, this same commenter recommended voltammetry or modeling work to identify a promising candidate before any additional work as done.

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

The reviewers disagreed regarding the adequacy of project resources. One reviewer indicated resources were sufficient, while another reported that resources were excessive. The first reviewer observed that the present funding was adequate, but should be increased when a suitable MAX candidate as identified for increased evaluation. The second reviewer acknowledged that while the project team did well with their funding to date, the likelihood of ending up with an energetic cell using these materials as anodes seemed very low. This reviewer expressed that it seemed a dead-end from a battery development point of view, and saw little reason to expect these materials to become viable as high energy or cost effective anode materials. Although these materials were interesting, this reviewer noted that funding this project could not be justified unless modeling data could indicate that the voltage penalty could be overcome or seriously mitigated.

U.S. DEPARTMENT OF ENERGY Renewable Energy

Synthesis and Characterization of Polymer-Coated Layered SiOx-Graphene Nanocomposite Anodes: Donghai Wang (Pennsylvania State University) – es147

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments in this section were generally positive. One reviewer stated that this program aimed at making core shell Si/C particles for the next generation of high energy batteries. Further, noted this reviewer, the approach was aimed at improving the cycle life and calendar life of such batteries. The second reviewer stated that Silicon anode materials offered promise for higher performance Li-ion batteries. The same person observed a very exploratory approach and acknowledged that the best technology had not been established.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Reviewer feedback, overall, was positive in this section. The first reviewer observed the following: design Sibased anode composite with fast kinetics, low irreversible losses, and tolerance for volume changes on charge and discharge; develop binders to improve



cycling stability, realized 200 cycles; and develop Si-based anodes with 40% first cycle loss and 90% efficiency. A second reviewer described the project team's approach, which included forming SiO_2 on the surface of Si, coating with C, and then dissolving out the SiO_2 . The reviewer added that this left a slug of Si within a hollow carbon shell to allow room for Si expansion while protecting the Si from the electrolyte that could otherwise lead to capacity loss from SEI layer formation and reformation. The second reviewer concluded that the only concern with this approach was that many other people have done, or were in the process of doing this.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Statements in this section were generally positive. One of the reviewers observed that the Si nanoparticles with controlled size and Si-graphene composites were prepared and characterized, new polymer binders were synthesized, and experimental electrodes were characterized. Another reviewer remarked that this project was quite new, but good progress was being shown after just a few months of work. The TEM imaging work done showed that the project team was making the core-shell structures it set out to make. This reviewer highlighted that the project team was already getting good capacity and decent cycle life (i.e., 2,500 mAh/g matrix for 80 cycles). The same reviewer opined that although this project had just started, more extended cycling work was needed.

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Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Overall, comments in this section were mixed. The first reviewer pointed out cooperation with PNNL (i.e., Zhang and Liu) and the Pennsylvania NanoMaterials Commercialization Center. The second reviewer stated this was unclear, but was unsure that much collaboration was needed.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Feedback was generally positive in this section. One reviewer listed the following: study SEI layer on Si-graphene and SiHC nanocomposites; synthesize and characterize amorphous Si-carbon nanocomposites; and identify causes of binder failure and designs of new low-swelling binders. A second reviewer explained that the plans seemed fine and expressed interest in seeing how the binder studies turn out. This reviewer concluded that more cycling work was needed.

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

The reviewers agreed that project resources were sufficient. The first reviewer observed these were adequate resources for the present study and suggested that the effort level should be increased if a breakthrough is realized. Another reviewer stated that the costs were modest.

Wiring up Silicon Nanoparticles for High-Performance Lithium-Ion Battery Anodes: Yi Cui (Stanford University) – es148

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer feedback in this section was positive. One of the reviewers remarked that this work was aimed at understanding the strength of Si nanowires and also ways to improve their cycle life. This reviewer continued that Si anodes were the most promising approach for the next generation of high energy density batteries. Another reviewer opined that Silicon anodes appeared to be the best choice for replacing graphite for higher energy storage capability.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project welldesigned, feasible, and integrated with other efforts? Comments were mixed in this section. The first reviewer stated that the major problem with Si anodes was the volume change on charge-discharge. This reviewer observed the following actions: it has concentrated on designing and constructing carbon nanotube anodes to produce a nano Si anode; it has developed a basic understanding of Si expansion and fracture during charge-discharge reactions of lithium; and it identified



hollow structures as a promising avenue for future work. Another reviewer acknowledged that the project team had taken a very nice, designed approach to try and accommodate the Si expansion by developing hollow nanowires of Si attached to a substrate. The Si could then expand inwards rather than outwards, which would expose less new Si surface to the electrolyte and minimize side reactions. The project team also had diffraction to study the reactive faces of the structures and had explored the impact of length and discharge rate on the fracture strength of these materials. This second reviewer, expressed uncertainty that nanowires, while exquisite and elegant, were ever going to be commercially viable, both from a manufacturing cost point of view and the space lost by relatively poor packing of the nanowire forests. The PI stated that the project team was going to start on more practical particles of Si, but nothing specific was outlined and it was unclear how relevant the work done would be to more practical materials. These materials may be useful to this program only for fundamentals studies; they are certainly very interesting, but this reviewer offered no chance of this type of work being relevant to anything but high cost batteries (e.g., microbatteries for electronics). This reviewer concluded that bulk materials were needed for large batteries, which could have nanofeatures.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

The statements in this section were positive. One of the reviewers observed potential for ten times the improvement over graphite anode materials. This reviewer continued that the PI had a history of taking the best course of action to solve problems, and

applauded the very prolific, cutting edge, research program. The reviewer also stated that double-walled nanotubes showed good promise and had given a long cycle life (6,000 cycles at 12°C Rate) and very high rate up to 20°C. Technically, asserted the second reviewer, this work had been very impressive. The SEM and TEM images had clearly shown that the project team has been successful in making the exquisite structures that were targeted and that the Si did indeed shrink inwards and partially fill the cores of the tubes. The double-walled hollow nanotubes worked very well, the pores were so narrow, and the aspect ratio so high that minimal Si/electrolyte reaction occurred inside these columns. This may have reflected either minimal electrolyte penetration into or maybe just minimal replenishment of the electrolyte inside the columns. Like others, the relatively low utilization of Si was actually a reasonable approach. This second reviewer further explained that while the 4,000 mAh/g was often used as the carrot, expansion and reactivity of a fully lithiated silicon anode would be very daunting to handle, especially for such long lifetime applications as electric vehicles. Thus, by backing off on the Si discharge, very high capacity could still be demonstrated while having a greater chance of assuring sufficient stability. With this method, concluded the same reviewer, the project team had attained very good cycle life (6,000 cycles and more) at a 1,000 mAh/g capacity.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Overall, feedback from reviewers in this section was mixed. The first reviewer recognized collaboration with many of the DOE BATT PIs as well as involvement with a number of universities and national laboratories. The second reviewer had not seen much evidence of collaboration, but noted uncertainty regarding the need for this if the project was only concerned with nanowires. This reviewer further explained that if the project team took its expertise and applied this to other, more practical Si materials, it would likely need to collaborate with other PIs, though many may view each other as competition.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments in this section were generally mixed. One of the reviewers listed the following: conduct transmission microscopy to watch Li-Si structure and volume change in real time in order to identify the best process for handling volume changes; take advantage of nanoscale designs to optimize Si anode structure; develop methods to produce designed experimental structure; and best experimental plan. The second reviewer emphasized that this work needed to be directed away from nanowires into more practical materials to satisfy program needs, and noted that it was unclear that this was going to happen, let alone how. The reviewer added that if the project team could not demonstrate a practical technical approach to truly viable materials, this reviewer asserted that funding additional work though the EERE program could not be recommended. Although the work on nanowires was really nice and elegant, this reviewer concluded that it was on the wrong material for this program.

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

The reviewers disagreed regarding the adequacy of project resources. One reviewer indicated that resources were sufficient, while another reported that resources were excessive. The first reviewer described the investigator as very prolific and having a knack for taking the best experimental approach to solve problems. Another reviewer observed an appropriate funding level. The same reviewer recognized that these were very hard studies to carry out and indicated the project team had been very successful on a technical level. However, unless the project team could demonstrate a clearer path to working on more practical materials, the second reviewer expressed fear that this work was of little practical benefit to the program. Until this could be done, the reviewer expressed inability to justify continuing program funds for this work. Perhaps, concluded this reviewer, the PI and project group were better focused on doing only fundamental studies. If so, this may be more appropriately funded out of the BES program.

U.S. DEPARTMENT OF ENERGY Renewable Energy

Synthesis and Characterization of Silicon Clathrates for Anode Applications in Lithium-Ion Batteries: Kwai Chan (Southwest Research Institute) – es149

Reviewer Sample Size

This project was reviewed by two reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Overall, statements from reviewers were positive in this section. The first reviewer indicated that batteries with significantly improved energy storage capability were essential to meet the demand for battery powered vehicles with ranges exceeding 200 miles. This reviewer continued that silicon anodes showed the best promise for increasing the energy storage capability of Li-ion cells, and that emphasis on silicon clathrates appeared to be a promising approach. Another reviewer expressed that this work was aimed at devising a clathrate structure of silicon that could form the basis of an anode material for the next generation of high energy density batteries.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Reviewer feedback in this section was positive. One of the reviewers opined that silicon appeared to be the best of many approaches. The second reviewer observed an



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excellent balance of both innovative and scalable methods to make silicon clathrates and also pointed out that parallel synthetic pathways had been evaluated by the project team. Moreover, this reviewer highlighted that the project team was very well aware of issues in devising a practical synthetic method and as not just developing a lab curiosity. The second reviewer also acknowledged the project team's firm theoretical understanding of the materials and processes.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments were generally positive in this section. The first reviewer observed that additive elements to stabilize Si clathrate structures had been identified. The same reviewer also stated that theoretical calculations and experiments gave consistent results. Another reviewer recognized excellent progress in making these new materials, and encouraged the project team to just do more in terms of characterization of the materials in cells. The project team showed good cycle life, but only at about 10% DoD (400 mAg/Si) and good capacity at one cycle. The same reviewer expressed that evaluating the wider range of performance and seeing how cycle life was affected by DoD is needed. This reviewer also described the sheer amount of work done in synthesis, characterization, and theoretical studies as very impressive, particularly in light of the modest funding level of this project.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Feedback from reviewers was generally positive in this section. One reviewer reported that Dr. C. Chan provided services for arcmelt synthesis of metal substituted clathrates, while Dr. J. Chen provided services and expertise on multi-anvil synthesis. The second reviewer observed that only a couple of PIs were working together, albeit very well. This reviewer opined that the project team could benefit from working with and deserve assistance from the national laboratories to help characterize the materials it was making.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments in this section were mixed. The first reviewer stated that the project team could carry out first principal calculations to identify the path for formation of empty clathrates of silicon, lithium-silicon, and lithium-silicon-X materials, while the second reviewer stated that the project team disclosed a very good plan going forward. This second reviewer underscored the need for the project team to evaluate the capacity/cycle life performance of its materials.

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

The reviewers disagreed regarding the adequacy of project resources. One reviewer indicated that the resources were sufficient and adequate. Another reported that the resources were insufficient, and that this was a very modest award. Additionally, this reviewer asserted that this project, both in light of the approach and results, should definitely continue or be expanded with both additional funding and direct support from the national laboratories in characterizing those materials in electrochemical cells.

U.S. DEPARTMENT OF ENERGY Energy Efficiency & Renewable Energy

Addressing the Voltage Fade Issue with Lithium-Manganese-Rich Oxide Cathode Materials: Anthony Burrell (Argonne National Laboratory) – es161

Reviewer Sample Size

This project was reviewed by five reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer statements in this section were positive. One reviewer strongly emphasized the relevance to DOE objectives, and another acknowledged that resolving this issue was critical to using these types of High energy materials. The third reviewer explained that for a successful utilization of Li-ion batteries in PHEVs and EVs, it was essential to enhance their gravimetric and volumetric energy densities, which, in turn, warranted new advanced electrode materials. High voltage, high capacity cathodes in the class of lithium and manganese rich NMC (LMR-NMR) cathode materials. $xLi_2MnO_3:(1-x)LiMO_2$ (M = Ni, Mn, Co), were quite promising. However, these materials underwent some structural transformation during the early stages of cycling that manifested as a voltage slump. As described by this third reviewer, the objective of this project are to mitigate such voltage slump by stabilizing open circuit voltage discharge profile during aging (i.e., voltage fade phenomenon) without sacrificing power, life, capacity, and abuse tolerance. Furthermore, offered the same

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reviewer, this would require a good understanding of and the mitigating of complex electrochemical-structural relationships of these materials, essential to successfully adopting this material in PHEV or EV batteries. The fourth reviewer commented that the goal of eliminating the change in the voltage curve for high-energy cathode materials was critical to getting this material to work. Such oxygen-loss materials were the only ones that could potentially provide higher volumetric energy cells (i.e., higher than high voltage LCO). Accomplishing this goal would help to provide a higher volumetric capacity, which would decrease cost, and decrease dependence on petroleum. The final reviewer answered yes, and added that the interdisciplinary team being assembled gave great hope for future developments.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Feedback was mixed in this section. The first reviewer observed that technical barriers were clear and well known, and highlighted that the reaction taking place during the first charge of the Li- and Mn-rich NMC cathode material had to be thoroughly investigated. Further, the capacity fade issue seemed to be the other important issue to be resolved. Another reviewer asserted that this could be the template for resolving other challenging problems, while a third reviewer remarked that a combinatorial approach to understand the phase diagram was an outstanding approach to sample the whole space and better understand it. Doing this right was difficult and would take a lot of focus, continued the reviewer. It was unclear whether modeling would help, but this reviewer pointed out that deep characterization would be very beneficial. Finally, the third reviewer reported uncertainty that a synthesis

approach would solve this problem. The fourth reviewer described the plan as solid and asserted the need for this program to sharply focus because of its significance to many material, battery, and vehicle manufacturers who were counting on this material to develop the next generation, low-cost battery. With the intention of not minimizing the significance of voltage drop, this reviewer relayed that discussion within the community pointed to life of this material as a more serious concern. Hopefully, concluded this reviewer, they were related intimately and the proposed work would resolve both the issues. The fifth reviewer recognized that the approach adopted here was quite broad and comprehensive starting with the following: definition of the problem and quantifying the limitations of the composite cathode materials; synthesis of a broad range of compositions of both lithium and transitional metals in combinatorial fashion through robotic means; fundamental characterization of these materials before and after aging using a suite of spectroscopic techniques; effects of surface coating and/or other treatments for a fix; detailed electrochemical performance assessment and its correlation to structural aspects; and augmenting the experimental findings with modeling and theory. The same reviewer noted that because this voltage fade was deemed the most important deterrent factor for using these materials, considerable emphasis had been placed on this project, with support from several individuals at ANL that contributed in the past to the development/understanding of these materials. Thus, explained the reviewer, all of the expertise at ANL was being brought into this project. The fifth reviewer described that one of the obvious problems with this comprehensive approach and broad trade space (in composition) was that too much variability in the results may be encountered without any clear correlations. Also, this reviewer added, the problem looked fairly daunting to be solved in a year. Lastly, this reviewer pointed out that the electrolyte, which was a key component in defining and determining the interfacial properties, was not part of those variables.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments in this section were mixed. Acknowledging that this was a new project, the first reviewer observed that there were not many accomplishments, except for the following: the problem had been defined; test protocols were established; and the team was formulated and the facilities identified for the synthesis, characterization, performance assessment, and post-performance characterization tests. In addition, this reviewer expressed interest that a more complete and comprehensive picture on these otherwise promising materials would emerge from these studies. The second reviewer also asserted that the project was just starting and noted difficulty in judging the technical accomplishments. Another reviewer agreed that it was difficult to judge the progress that has been made because the program was in its infancy. The fourth reviewer indicated this was not really applicable at this stage, though there may be difficulties with only using the combinatorial approach. This reviewer suggested giving thought to a secondary synthesis approach, and at least check on promising results. The final reviewer reported no progress shown beyond scoping the team and problem.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewer statements were generally positive in this section. One of the reviewers described the team as strong and of great quality, and another observed a good collaborative team. The third reviewer noted multiple team members and collaborators from ANL, which was expected because of the nature of the project. However, considering the complexity of the problem, this reviewer suggested that it would be prudent to go beyond ABR to address these issues. The fourth reviewer explained that while it probably was already in the plan, involving actual material manufacturers (e.g., battery makers at least) would be desirable. The fifth reviewer agreed that progress would be faster if the project team could find a way to work with a major material supplier. This reviewer also asserted that the model of this approach was collaboration.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Comments received in this section were generally mixed. The first reviewer noted great direction and suggested focusing on the phase diagram. Understandably, remarked the second reviewer, future plans were aimed at understanding the cause of voltage fade and constituted the following: selecting the most promising compositions/chemistries for exhaustive electrochemical evaluation; characterizing their chemical, physical and thermal properties; correlating with electrochemical properties; and evaluating the electrodes in a full lithium-ion cell configuration, hopefully with reduced voltage fade. Another reviewer reiterated that the work

plan looked solid, but cautioned that while using materials synthesized by various processes was understandable, the authors should eventually focus on a synthetic procedure that emphasized low cost. Otherwise, continued this reviewer, it would be back to the drawing board. The fourth reviewer asserted that communication between the different team members was going to be critical. This reviewer opined that, in terms of modeling and theory that the authors have proposed, it could be of great interest if the project team managed to provide trends and useful hints to the experimentalist. Although the absolute values may be off slightly, the reviewer observed that trends could provide very useful information. Finally, this reviewer observed that the synthetic work seemed to become very important. The fifth reviewer recognized that these materials also had an initial gassing issue, and that the project team should probably address this simultaneously.

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

The reviewers disagreed regarding the adequacy of project resources. Three reviewers indicated resources were sufficient. One of these reviewers further stated that the institutions involved seemed to be well-equipped, while another remarked that ANL had the best lab in the world for Li-ion materials development. The third reviewer pointed out that additional funding may be necessary if results looked promising and if there was a need to resolve this issue more quickly. The fourth reviewer reported that the resources were insufficient and recommended adding more funds to this project because of its high importance. The final reviewer observed that the budget looked a little excessive, but the complexity of the project probably justified it.

Development of Industrially Viable Battery Electrode Coatings: Robert Tenent (National Renewable Energy Laboratory) – es162

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Mixed remarks were received in this section. One of the reviewers described energy storage as an important issue in the electrification of transportation necessary to reduce petroleum imports. Another reviewer indicated that the relevance depended on the success of the program, and that while it has not yet been shown that continuously applied coatings would result in improved performance, this program may provide that information.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Overall, reviewer feedback in this section was positive. The first reviewer observed an interesting project with great potential for significant advances, and a second reviewer asserted that integrating ALD into an electrode manufacturing process was attractive both from the cost and performance aspects. The final reviewer indicated that the program was setting up to do an automated line without doing many preliminary experiments, and



continued that the problem was reflected in the results of 18650 cells made at Sandia that demonstrated a number of cell failures. This third reviewer also highlighted that the heat of reaction of charged cathodes was worse for the coated electrode than for the uncoated, although the onset temperature of reaction was slightly lower for the uncoated. The reviewer expressed the belief that it would be cost-effective to demonstrate good results with a single coating head before going on to design and implement a multiple head continuous process.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments in this section were generally positive. One reviewer reported significant progress shown in technical advances to date, while a second reviewer offered that the results on Si carbon seemed to be better than those on $LiCoO_2$ and other high voltage materials. Although this project started only recently, the third reviewer observed good technical progress. Basic feasibility was demonstrated and prototyping was under way to improve original design. This reviewer further noted that the quality of the figure shown on Slide 7 was poor and it was hard to distinguish between items. Regarding the ALD coating applied onto an electrode slurry coated foil, this final reviewer inquired about the uniformity of this coating – whether its location was restricted to the top surface of the electrode power layer, or whether the coating was uniform throughout. The reviewer explained that it would be useful to understand this as this may help optimize the process to maximize benefit. In conclusion, this reviewer suggested that
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cross-sectional analysis may help understand this, and that one would think applying ALD on powder in some sort of fluidized bed would result in a more uniform coating than coating on the electrode.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Statements from reviewers in this section were mixed. The first reviewer stated the collaborations were very appropriate to the goals of the project, while the second reviewer strongly recommended partnerships with other academic institutions that made single crystalline, nanoscale materials for electrodes. This reviewer explained the recommendation by stating it was easier to understand the role of protective coatings on many of these electrode materials.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Feedback was somewhat negative in this section. One reviewer described the proposed activities as reasonable. Another reviewer expressed desire to see a concentration on Si electrodes because they seemed to show the best results. This second reviewer observed no discussion during the presentation of which electrodes would be studied in the future, and pointed out that an early success with one electrode would be significantly more impressive and prove the method better than a slower program trying to establish results for several electrodes.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? The reviewers agreed that the project resources were sufficient.

Design of Safer High-Energy Density Materials for Lithium-Ion Cells: Ilias Belharouak (Argonne National Laboratory) – es163

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Reviewer feedback in this section was positive. The first reviewer indicated this work provided ANL with a scaleup capability for its new materials and was essential to developing its in-house materials both in terms of making larger samples to enable a more in depth evaluation of the high energy materials, and to help promote manufacturability of the new materials. Another reviewer stated that yes, high energy materials were critical to the objective of petroleum replacement, while a third reviewer asserted that this study was required so that optimal compositions could be determined. The final reviewer explained that batteries could help with electrification of the transportation sector and reduce petroleum imports.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts? Statements in this section were generally positive. One



of the reviewers observed a logical, sound approach, and another reviewer described the approach of using a CSTR-type reactor for co-precipitation as interesting. The third reviewer agreed that the approach was interesting, and expressed hope that the team manages go all the way towards cell fabrication and scale-up. Additionally, continued this reviewer, the project had an important mixture of very basic science and vastly applied research. This reviewer finally communicated that it was envisioned that the project team was also going to be well-integrated with other efforts from NRL. The final reviewer noted it was a decent approach and very good characterization tools were being used by the project team. Although this same reviewer agreed with the combinatorial approach to exploring the landscape of materials, this reviewer would have thought this was something that could have been framed out to Wildcat Technologies rather than bringing it in-house. Further, Wildcat Technologies was already set up to do similar work and had been pretty successful to date.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Overall, positive feedback was received in this section. One of the reviewers observed significant progress in a short time, but another reviewer cautioned that it was hard to judge at this early stage. This second reviewer acknowledged that the carbonate precipitation and growth mechanism that seemed to go out of control a little was interesting, and opined that the hydroxide precursors seemed to be the way to go for these high energy density materials. The third reviewer reported that this team investigated co-precipitation technique and its scaling for increasing materials production using CSTR-type reactors. Primarily, the

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project team identified some issues related to the processing and resulting materials characteristics. This same reviewer indicated that the PI wanted to address this technical barrier by looking at the gas phase technique for producing these materials, and agreed that this should be explored. This third reviewer highly recommended using gas phase techniques to prepare these mixed metal oxide particles. In conclusion, this reviewer recognized that these methods could be highly scalable and cost-effective. The final reviewer stated that finding gaps in some materials and identifying that these could lead to fracture during calendaring was noteworthy, and that the nanoplatelets also looked interesting. Although the project team could make different structures, this reviewer expressed uncertainty that the team fully understood those processes yet.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments in this section were somewhat positive. The first reviewer stated good, and a second reviewer acknowledged the team had some partnership with an academic institution regarding gas phase synthesis. This second reviewer strongly recommended that the team seek some partnership with other established groups specializing in gas phase production of materials. Another reviewer opined that collaboration with industry would be important at some point, particularly if the practical aspects of the materials were demonstrated. The final reviewer observed good imaging work and collaboration within the national laboratories, but would have liked to see more interaction with commercial materials companies such as BASF.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Overall, reviewer feedback was mixed in this section. One reviewer praised the description of future work as well thought out, and noted that the synthesis with hydroxide of spherical particles was impressive for hydroxide. This reviewer further offered that stabilizing carbonate particle size may eliminate some of the problems. Another reviewer stated that the planned work involving a gas phase production technique and improving the co-precipitation technique was reasonable. The third reviewer indicated the project team's plans looked fine, but would have liked to have seen more work done to develop and characterize the material produced by the spraying technique. The same reviewer questioned whether the project team was best suited to do the combinatorial exploration, and saw no reason why it could not do this given more time and money. Furthermore, this reviewer did not expect such work to lead to the cause of the voltage fade with the ANL layered material, although it may have an effect. This reviewer opined that understanding would be expected to come from additional, in-depth characterization of the existing materials; any improvements from the combinatorial approach would likely be empirical, rather than fundamental, in nature. The final reviewer remarked that the aerosol particles could be an interesting approach, but noted that the aerosol particles may be of low tap density. Additionally, the reviewer recommended that the authors should, at some point, report their capacity data in terms of mAh/g total electrode weight rather than only active material weight.

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

The reviewers agreed that project resources were sufficient. One reviewer observed the project team was doing well with modest funding. Another reviewer opined that resources may be insufficient if the team managed to make a lot of progress during the year, and that the team may need additional support if the practicality of these powders was demonstrated.

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Overcoming Processing Cost Barriers of High-Performance Lithium-Ion Battery Electrodes: David Wood (Oak Ridge National Laboratory) – es164

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments in this section were positive. The first reviewer indicated that developing an aqueous-based anode and cathode coating process could reduce the cost of Li-ion batteries and the capital equipment to set up new facilities. In addition, the reviewer opined that it was significantly better, environmentally, because it eliminated the use of a somewhat toxic solvent. NMP. Another reviewer observed the relevance was to low cost electrode manufacture, which had an important effect on cell costs. This reviewer pointed out that use of a polysaccharide for the cathode binder was problematic, however, because of the high positive potential applied to this electrode during charge and storage. The same reviewer stated that the additive (PEI) was an easily oxidized compound. Finally, this reviewer remarked that these hydrophilic materials were also known to hold water and the temperature needed to completely remove adsorbed water without dehydrating the polymers it is unclear.

Question 2: What is your assessment of the



Overall, feedback in this section was mixed. One of the reviewers thought the work was extremely well designed and particularly appreciated the science and methods used to design the process rather than the often used empirical approach. This reviewer explained that water-based coatings for anodes were becoming quite common in industry, but cathodes were still mostly made using NMP solvent. Thus, the reviewer stated that this project addressed a real need. This reviewer praised the project team for working on the cathodes first. Another reviewer opined that replacing NMP with water-based chemistries had huge potential to simplify and reduce the cost of making cells. The third reviewer indicated that the approach should take into account the possibility of carrying adsorbed water into the cell as well as of oxidizing the binder and/or additive. Additionally, this reviewer emphasized it was also important to determine adhesion and cohesion of the materials to the electrode and that these tests should be run routinely with new binder systems. This reviewer further remarked that hydrophobic binders should also be tested as there were a number already in the patent literature. This reviewer opined that the effort should be to test electrodes in finished cells and the facility at ANL to make 18650 or pouch cells should be utilized to test these electrodes in finished cells. Ideally, continued this reviewer, the conventional binder should be used on one electrode while the trial binder was used on the other electrode. In closing, this final reviewer asserted that cycling tests in coin cells were unacceptable measures for coating validity.

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Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewer feedback in this section was somewhat negative, overall. The first reviewer was very impressed with the project team's overall progress to date and looked forward to the project team's next debrief. This reviewer stated the project team's zeta potential work highlighted the desirability of using a cationic surfactant. Using surface energy measurements, the project team set clear goals for what it needed in terms of aluminum surface energy and by using corona plasma treatment. Thus, the project team identified key problems and found solutions to both. While the project team did not have time to go into details, this reviewer recognized that it had an appreciation of the importance of mixing order and processing. This reviewer pointed out that the project team did not yet have an understanding of what the corona treatment actually did, but the project team had only been working on this for a very short time. The same reviewer suggested that it would have been helpful to include more direct comparisons of their results with NMP coated electrodes (e.g., visual appearance, etc.), and to revisit and compare the binder choice to SBR and CMC. Recognizing the difficulty in getting such details into such a short presentation, this reviewer assumed that water removal was not a big deal as compared to NMP, but suggested it would be good to see that spelled out in the future. The second reviewer stated that it would be useful to compare the viscosity of NMP versus water-based slurries for different total solid loadings because NMP enabled very high, solid loadings that enabled high throughput coating. This reviewer inquired as to the following: whether the same could be accomplished with water-based slurries; whether it was harder to disperse anode and cathode particles in a waterbased slurry; whether higher energy dispersion needed to get the same level of dispersion as for NMP; whether longer dispersion time was needed; and whether drying time with a water slurry was significantly longer as compared to NMP slurries. The same reviewer recommended showing side-by-side results for NMP-based slurry when presenting surface energy measurements, and further suggested that the C-rate studies would be helpful in understanding the quality of dispersion and electrode as a high C rate would magnify any potential issues with electrode quality. The final reviewer observed that the disastrous results with 1.5% PEI were not explained, but this was a concern because if a mistake was made in coating, it implied that only a single electrode was tested. The reviewer added that it should be standard practice to use multiple electrodes of the same formulation to measure these properties. In conclusion, this reviewer stated that the electrodes should be tested in sealed cells for adequate measures of cycling and the LFP cathode should show no fade after 50 cycles to be acceptable.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Remarks were mixed in this section. One reviewer remarked that the project team seemed to be well connected and liked the electrode sharing among the labs for independent evaluation and feedback to the PIs. This reviewer suggested that the project team line up with a battery maker to see if it was interested in evaluating the project team's process and/or giving feedback regarding the quality of electrodes that this group was making. Another reviewer wanted to see a coating company or coating expert brought into the program to provide guidance to the team on battery electrode formulation, mixing, and coating.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Reviewer feedback in this section was generally negative. One reviewer suggested the team work with cell builders at ANL and SNL to determine the proper electrode thickness and loading for measurements in full cells. While the processing aid (PEI) should not affect the anode, the second reviewer encouraged the project team to get an evaluation in full cells as soon as possible in case the project team got an unexpected adverse interaction. Although it was currently slated to be done by September 2012, this same reviewer recommended that the project team jump ahead and do a rough check for unknown problems while doing the more methodical work planned. This reviewer also suggested that the project team get a better understanding of what the corona treatment was actually doing to the aluminum, through such means as surface roughness and maybe FTIR/ESCA studies. The project team should validate the corona method by using Al foil from a different vendor, although this reviewer believed that this would not be a problem. It was also suggested by this reviewer that the project team examine its coatings at the edges to see how clean they were. The reviewer reported that this was generally a critical QC metric in electrode fabrication, especially if using a pattern-coated system often required for commercial electrodes. Wetting of the mix could be critical in controlling this edge effect, emphasized the reviewer, and if it wets too well, one could get smeared out edges rather than sharp edges. This final reviewer

further recommended that the project team try and run the line at high line speed settings, although the project team could not be expected to mimic commercial production in its lab.

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

The reviewers disagreed regarding the adequacy of project resources. Two reviewers indicated that resources were sufficient, while another reported that resources were insufficient. One reviewer observed that it was an appropriate funding level and the project team was getting good results with it. Another reviewer suggested an electrode team of several DOE labs and industry experts would be most useful as a resource for this project.

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Roll-to-Roll Electrode Processing and Materials NDE for Advanced Lithium Secondary Batteries: Claus Daniel (Oak Ridge National Laboratory) – es165

Reviewer Sample Size

This project was reviewed by three reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback was somewhat positive in this section. One of the reviewers reported that non-destructive evaluation was already used in the battery industry for electrode manufacture, and that this program intended to improve the analysis to permit higher product yield (i.e., a lower scrap rate) for the process. A lower scrap rate, explained this reviewer, meant lower costs as the scrap electrodes were expensive and not easily recycled. The second reviewer stated the objective was not clear, but this could be part of the program, though. Further, continued this reviewer, defining the quality of what was bad or good (i.e., criteria for passing or failing) is needed. The same reviewer commented that without these criteria, it was difficult to discuss the cost by increasing the electrode yield.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project welldesigned, feasible, and integrated with other efforts?

2.50 2.00 1.50 1.00 0.50 0.00 Approach Tech Collaboration Future Research Accomplishments Relevant to DOE Objectives Sufficient (100%) Yes (100%) Reviewer comments in this section were generally mixed. The first reviewer opined that relatively small changes in Li/(Ni+Mn)

ratio could significantly influence performance of the cell, then queried whether methods described in this work achieved the resolution that would be needed. Another reviewer stated the approach was generally good as the methods suggested were capable of high accuracy. The same reviewer noted that the comparison to existing beta detectors was not included in the approach to the work, and suggested that this was an oversight. Additionally, continued the second reviewer, the means of fairly assessing the laser ranging or the XRF methods to actually reduce scrap rate was not clear. A full production demonstration would seem to be required, but no discussion on this was proposed. This reviewer reported that, at present, the simplest form of electrode making (i.e., tape casting), was employed for the evaluations, but no comparisons had been made. The third and final reviewer identified a need to determine the current quality check being done for the electrode production and address why this approach could achieve the objective. The same reviewer requested clarification regarding why an IR imaging and laser system was better or could achieve the objectives as compared to the industry standard vision and x-ray (Beta ray system) in terms of resolution and detecting speed. Finally, this reviewer recommended verification that the XRF had capability to check with the line speed of 60m/min.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Remarks in this section were generally negative. One of the reviewers observed that the thickness measurements displayed a high degree of inaccuracy on which the authors did not comment. XRF did not seem to show any deviation in composition, which was a

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good result. The IR imaging seemed to show inhomogenieties, but no comparison to production electrodes was made. The second reviewer stated it was believed that TEM and XRF can analyze the level of powder, but should be too much at the electrode level. Also, the increase in the electrode yield should be conducted on the step of mixing and slurry making process.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Comments were generally negative in this section. The first reviewer indicated the program would benefit from working with groups that actually do electrode manufacture intended to mimic industrial practice. Another reviewer pointed out the need to investigate the current SOA technology for the quality check of electrodes.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Feedback from reviewers in this section was generally negative. One reviewer suggested that the group attempt to compare actual weight loadings to thickness as measured by the laser ranging system, while the second reviewer reiterated the need to resolve issues stated previously in response to the questions above.

Question 6: How sufficient are the resources for the project to achieve the stated milestones in a timely fashion? The reviewers agreed that project resources were sufficient.

Post-test Cell Characterization Facility: Ira Bloom (Argonne National Laboratory) – es166

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Feedback was positive in this section. The first reviewer explained that this new facility was built to be a central point for studying lithium-ion and other advanced automotive batteries and their morphology after the batteries have aged for USABC and DOE-funded projects. The goal, as indicated by this reviewer, was to understand the factors behind the decline of battery performance so that this knowledge could be implemented in improved battery designs. This reviewer concluded that improving the lithium-ion battery chemistries used in plug-in electric vehicles (PEVs) would encourage consumer adoption of PEVs, which would help to displace petroleum. The second reviewer highlighted the significant need for independent evaluations of new technology developments, and opined that this facility should speed the adoption of new Li-ion and other battery/fuel cell developments. Another reviewer asserted that this was a very useful system for post-test breakdown and analysis. The fourth reviewer remarked that this capability was pretty important to understand the mechanism for capacity fading and impedance growth.



Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Comments were generally positive in this section. One reviewer opined that the system had been well thought out and appeared capable of outstanding evaluations of cell operations. Another reviewer acknowledged ANL's long history of battery testing, which goes back to the 1970's, while a third reviewer recognized that a central facility for this purpose of testing batteries to understand the reasons for their decline was new for the ABR program at ANL. The third reviewer further expressed that an entire suite of equipment to perform the diagnostics had been acquired, and applying a more standardized approach of tests to the various types of battery chemistries submitted to the facility should yield datasets that could be used as benchmarks as battery development in the DOE-funded programs continues. The final reviewer recommended that the gas analysis be combined with the post-test capability and storage test, etc.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Reviewer feedback was generally positive in this section. The first reviewer pointed out that after 18 months of development and funding, the facility successfully opened in January 2012 and was already providing the kind of analysis on aged batteries that it was built to do. From here on out, reported this reviewer, it would be a continuously operating facility. Another reviewer stated

that results on tested cells had been very informative and the analysis methods were state of the art. The third reviewer described the wide range of instrumentation and test equipment as essential. The fourth reviewer remarked that other supporting data, as well as XPS, could be shown.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

The comments received in this section were somewhat mixed. One of the reviewers observed the facility was open and had capability to carry out capacity tests, electrode segmentation, analysis of particles of active materials, etc. Another reviewer acknowledged that as a central facility for the national laboratory groups that were investigating lithium-ion batteries and the chemistries beyond lithium-ion, much of the value of this lab lay in its ability to serve the projects coming out of the ABR, BATT, and USABC programs at ANL and other national laboratories. The final reviewer suggested that the more specific objective should be set up for analysis with the specific cell chemistry, and further recommended that this facility be more open to cell developers.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

Feedback from reviewers in this section was generally positive. One reviewer indicated initial plans seemed well-chosen and explained that the lab served as a facility, so the general plan was for it to analyze batteries that have already been through the standard testing procedures conducted in other labs. Additionally, continued this reviewer, the purpose of this lab as a final stop for analyzing these batteries was quite clear and straightforward. The second reviewer stated it would continue to provide a service to the DOE battery R&D efforts as well as outside requests.

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

The reviewers agreed that project resources were sufficient. One reviewer stated resources were adequate for intended service. Another reviewer noted that while the initial \$2 million given to the lab was clearly enough to get it set up and running, funding would presumably be coming out of a different pathway now because it would be operating as an ongoing facility now.

Process Development and Scale up of Advanced Cathode Materials: Greg Krumdick (Argonne National Laboratory) – es167

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Comments in this section were positive. The first reviewer stated that new materials program needed a scale up facility of this sort to accomplish DOE goals. It was stated by another reviewer that the scale up was important for process development. The third reviewer observed that a facility to provide a systematic engineering approach to scaling up the production of lithium-ion battery cathode materials from the small quantities required for laboratory bench research had been a missing link for batteries developed by the Vehicle Technologies Program (VTP), according to the PI. The reviewer opined that this program would help industry make decisions as to whether to invest in technologies developed in the program, so that the most promising technologies would become commercialized. Making top-performing lithium-ion batteries that would make plug-in electric vehicles (PEVs) reliable and safe would encourage sales of those vehicles and therefore displace some of the internal combustion engine (ICE) vehicles that use petroleum. The final reviewer



explained that DOE was charged with developing new battery and fuel cell systems capable of competing with the present gasoline powered vehicles. That required new battery and fuel cell chemistries and systems. The key element in this process was the ability to demonstrate feasibility of the new systems on a commercial scale. This project, continued this reviewer, represented the first stage in validating a new system, which required pre-commercial process development for new materials and the capability to assemble commercial prototype cell products.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Feedback from reviewers in this section was generally positive. One reviewer indicated that the challenge of scaling up the production of materials for batteries was not one that had been seriously addressed by the VTP battery research programs thus far. This reviewer further explained that this program was very serious about filling in this gap, and the new facility had acquired specialized equipment from Japan and Korea, as well as hired two full-time specialists who had knowledge in this area. The second reviewer opined that the scale up seemed well within the guidelines of a good chemical scale up facility. This reviewer also observed the construction of a reasonable size dry room and the capability to produce pre-commercial quantities of the active materials and components for evaluation. While not yet complete, this project was a key element in finding and qualifying a new technology for further commercial validation. At this stage, remarked this reviewer, it was essential to be able to produce 500 to 1,000 experimental cells to identify the optimum condition to produce the new cell materials, but also to assembly the cells. This

reviewer also stated it was necessary to represent on a statistical basis matching the performance forecast in the research process. Because little infrastructure existed in the United States for Li-ion cell manufacturing equipment, other resources may need to be imported to satisfy the need for experimental samples. The third reviewer asserted work was needed on other process development that the other companies and institutes were working on.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments in this section were mixed. One of the reviewers explained that the new facility has so far scaled up one lithium-ion cathode material up to a certain level, and it is in the process of scaling up the production of this material to the kilogram scale. The group has created a process for identifying the materials that should be scaled up, and once it achieved the optimized process for scaling up production, the team would produce technology transfer information packages to make this knowledge available to companies that may wish to license the approach, as well as kilogram-scale quantities of sample materials for evaluation purposes. It was noted by this reviewer that such a facility was absolutely needed because coin cells (i.e., the sort of cell one is limited to making when working with laboratory-scale amounts of materials) did not give enough information on how a product would work when scaled up for a PEV. The second reviewer reported that the tests seemed valid so far for scaled up high manganese materials. However, this reviewer cautioned that coin cell tests were not sufficient and should be backed up with full cell tests. The same reviewer pointed out that cost estimates would probably be somewhat crude because these were only pilot line scale up experiments, but stated that at least some guidance should be available. Another reviewer opined that progress had been slower than desired to meet the goals set by the DOE program. Although this reviewer acknowledged that the materials preparation was being proven, it was noted that the cell assembly capability was not yet in place. Once it is in place, it will require four to six months to prove-in the cell assembly capability, which this reviewer described as a slow time line that would not be tolerated in industry. The final reviewer stated it was well defined to the ANL cathode powder process, but suggested to develop the process that was made by the other companies or institutes. The same reviewer also identified the need for the testing and diagnostics team to set up clear criteria to determine whether to go (or not) for scale up.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewer feedback was generally positive in this section. The first reviewer remarked that it was unclear that much collaboration with partners was needed to get this facility underway, but suggested that it would probably benefit, going forward, from collaborating with the laboratories that were testing new sample materials. The second reviewer observed that materials and cell assembly seemed to be inward looking problem areas. Once fully operational, this reviewer asserted, collaboration with other institutions should follow.

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The comments received in this section were mixed. One reviewer indicated that the cathode materials research and scale-up facility expected to do two to four materials in the coming year. The approach appeared sound to this reviewer, even though the facility would be relocating shortly, which would briefly hinder its progress. Another reviewer opined that the time frame for this essential facility was to the detriment of the ANL and DOE materials programs. Efficient and timely (i.e., the sooner the better) evaluation of new materials would benefit the entire ANL materials program, concluded this reviewer.

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

The reviewers disagreed regarding the adequacy of project resources. Two reviewers indicated the resources were sufficient, of which one of further indicated the resources looked sufficient to cover the costs of the equipment as well as that of two full-time engineers with specialized skills in materials production scale-up. The third and fourth reviewers reported that the resources were insufficient. The third reviewer opined that more funding was essential because cell assembly and materials preparation required capital and qualified engineers to execute the program in a timely manner. The fourth reviewer observed the need to hire more operators to accelerate the pilot production.

Process Development and Scale up of Advanced Electrolyte Materials: Greg Krumdick (Argonne National Laboratory) – es168

Reviewer Sample Size

This project was reviewed by four reviewers.

Question 1: Does this project support the overall DOE objectives? Why or why not?

Overall, comments in this section were positive. The project supports the creation of a facility to develop processes for scaling up the quantities of electrolyte materials for lithium-ion batteries that are used in plugin electric vehicles (PEVs), as indicated by the first reviewer. If lithium-ion batteries with improved performance and safety properties could continue to be developed and commercialized at reduced cost, opined this reviewer, this would help speed up consumer adoption of the PEVs that use these batteries. Many of these PEVs would surely replace the purchase of conventional vehicles that run exclusively on petroleumbased fuels and thus, this reviewer asserted, the project did support the DOE objective of displacing petroleum. The second reviewer explained that advanced lithiumion chemistries with high energy densities were the horizon for PHEVs and EVs, aided by the rapid emergence of new materials for cathodes, anodes, electrolytes, and electrolyte additives for interfacial stability or over charge protection, both within the DOE



laboratories and elsewhere. In addition to the performance improvements with these materials, this reviewer continued, these materials' cost purity and manufacturability were also important factors in the overall cost, life and feasibility of PHEV batteries. The objective of this project, per this reviewer, was to develop scalable processes for manufacturing electrolyte materials, synthesize kilogram quantities of each material, and make them available for industrial evaluation in large-format cells. The second reviewer remarked that this program was a key missing link between the discovery of advanced battery materials, market evaluation of these materials, and high-volume manufacturing, and would also reduce the risk associated with developing and maintaining a domestic, commercially viable, battery manufacturing capability. Another reviewer claimed that, as per the presentation, the project provided a vital link for electrolyte development and improvement that had been missing. Furthermore, noted this reviewer, it appeared that ANL was willing to underwrite this activity as the funds provided clearly did not cover what was being done. The fourth reviewer answered with a cautious yes stating that electrolyte research was critical to the ongoing evolution of battery technology, which was an important factor in petroleum displacement. Beyond the technical merits of a potential electrolyte material, continued this reviewer, it was also critical that the proposed technology had the potential to scale both in volume and cost in order to be considered a legitimate option in the battery development path. This reviewer expressed concern whether a DOE-sponsored program could have the breadth and scope capable of positively impacting the commercial viability of electrolyte materials. On the one hand, described this reviewer, it would seem that if an electrolyte material, whether it was salt, additive, or solvent, was demonstrated to have significant technical advantage, the industry would work diligently to determine if it had commercial viability. What this reviewer questioned was whether an intermediate role within the DOE was

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either necessary or sufficient to provide a bridge or incentive to commercialization. The reviewer affirmed that this was not a passing of judgment, but rather a simple note that a program such as this probably required very careful, ongoing evaluation to determine its relevance within the overall scope of battery materials development.

Question 2: What is your assessment of the approach to performing the work? To what degree are technical barriers addressed? Is the project well-designed, feasible, and integrated with other efforts?

Feedback from reviewers in this section was generally positive. One reviewer stated the approach appeared to be logical and well thought out within its scope and mission, while another reviewer indicated that the approach was excellent. This second reviewer suggested that while more description of the analytical specifications and methods would improve the confidence, most of the bases were generally covered. The reviewer concluded that future testing of the materials would reveal whether the analytical and quality control was adequate. The third reviewer remarked that this electrolyte scale-up facility had established a procedure for how it would select which electrolyte materials to develop scale-up processes for. This reviewer further described that the facility staff included scale-up experts who knew how to develop the processes that would allow cost-effective volume-scale manufacturing of these materials. After going through two rounds of scaling up to arrive at the ability to make kilogram-scale quantities of the materials, the reviewer pointed out that the team would write up a technology transfer information package that would be available for licensing by industry. So far, acknowledged the third reviewer, five materials had been successfully scaled up. The fourth and final reviewer reported that the approach for scale up of the selected electrolyte materials, which looked good, involved the following: identifying the desired materials (i.e., electrolyte solvents, redox shuttles, and passivation additives from the ABR material development; developing and managing the materials database, which includes chemical identity and performance characteristics; developing rating criteria (i.e., rate, life, and overall performance; developing a cost-effective, scalable, and safe manufacturing process together with analytical methods and quality control procedures; iterative synthesis and performance validation; creating a detailed technology transfer package; and making the material available for use by industrial partners. This final reviewer expressed it was unclear why the scale up should be limited to the material from ABR only, and added that any promising materials emerged from the external partners should be scaled up to be able to verify the performance befits with such materials in large-format cells containing ABR chemistry.

Question 3: Characterize your understanding of the technical accomplishments and progress toward overall project and DOE goals.

Comments in this section were mixed. One of the reviewers described the progress as excellent and accomplishments as very concrete. Another reviewer reported that the facility has thus far reported that five electrolyte materials have been successfully scaled up at the facility. It has also worked on another material that ultimately it deemed unsuitable for scale-up. The reviewer further indicated the facility maintained a database of prospective materials for scale-up, and it appeared that this catalog would help it in deciding which materials to work with next. The third reviewer observed that reasonably good progress had been achieved thus far in developing synthetic processes and synthesizing large batches (kg) of five electrolyte materials, which include four new solvents/redox shuttles from ANL and one electrolyte additive, hexafluoro-iso-propyl phosphate (HFiPP) from ARL. During the synthesis, explained this reviewer, some of the environmentally not-so-friendly solvents were replaced with green alternates and the process waste was reduced. Technology transfer packages were prepared for these materials and materials were sampled for evaluation. It was not clear to this reviewer why the material selection could not be extended beyond the ABR materials. Also, pointed out this reviewer, plans regarding the project team's subsequent evaluation in large-format cells through industry collaboration were not discussed. Nevertheless, the third reviewer concluded that scale-up efforts in this project were in the right direction to enable and expedite technology transfer from laboratory to industry. The final reviewer commented that it would have been good to get some details of how the data generated from the scale up sample matched the original discovery material. Finally, this reviewer highlighted that there were no examples of data back from scientists or industrial feedback from samples that were distributed.

Question 4: What is your assessment of the level of collaboration and coordination with other institutions?

Reviewer feedback was somewhat negative in this section. The collaborations were limited to two ANL teams and the United States Army Research Laboratory, reported the first reviewer. However, the reviewer continued, facility management was aware that more collaboration was necessary and was actively soliciting the participation of research groups within the ABR program

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community. The second reviewer remarked that, as expected from the nature of the project, there were a few contributors and collaborators to provide electrolyte materials. This reviewer further highlighted this needed to be extended to external collaborators beyond ABR and industry. As another reviewer noted from the presentation, the collaboration sphere needed to be expanded on both the material source as well as the ultimate evaluators of the materials. At the same time, this reviewer pointed out that the process technology necessary to develop any given set of materials might be quite different from the process technology developed from a previous campaign. This reviewer suggested it would be good to be able to access subject matter experts in any given process development rather than to try and build the expertise from the ground up. The fourth reviewer observed an obvious need to do better here and emphasized that vaguely offering to collaborate with ABR participants was inadequate. The same reviewer identified a clear need for a salesman and further inquired about the existence of collaborations with chemical manufacturers (e.g., Aldrich, Novolyte, etc.).

Question 5: Has the project effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology, and, when sensible, mitigating risk by providing alternate development pathways?

The comments received in this section were generally positive. One reviewer stated the approach that the electrolyte materials scale-up facility had developed seemed logical, and with the input of research groups that focus on these materials, it should be able to choose the most promising electrolyte materials for its future efforts in process development. Not all materials may be able to realize the same degree of success in achieving cost savings and simplified processes for volume manufacturing, but this reviewer observed that the team appeared to be off to a good start thus far. Having a facility of this type was very valuable to the ABR program, opined this reviewer, as scaling up materials for volume production was a missing link between the industrial evaluation of material and their commercialization in batteries for PEVs. The second reviewer reported that future plans, which were in tune with the overall objective, included managing the electrolyte materials. Another reviewer explained that future plans involved moving into new facilities, which was a bit vague. Future activities would obviously depend on deliveries next year, continued this reviewer, who also pointed out that this would be critical and would then require more concrete plans for improving the processes. The fourth reviewer offered no comment, beyond having observed that it essentially involved moving forward with developing more compounds.

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

The reviewers disagreed regarding the adequacy of project resources. Two reviewers indicated that the resources were sufficient. The first of these reviewers remarked that funding appeared to be sufficient, supporting the acquisition of the appropriate equipment and staff with the skills to develop the processes for manufacturing electrolyte materials at volume scale. The second reviewer agreed that resources seemed sufficient for the task, and further noted that this may vary depending on the forward going nature of the specific materials in question. Any level of commitment to scale up technology would require significant funds, opined this reviewer, and the breadth and scope of such an effort would be a complex issue for which to manage and provide resources. Another reviewer reported that resources were insufficient and expressed that the project was clearly underwritten by ANL funds. In addition, this reviewer emphatically expressed hope that the amount of the subsidy was being relayed to the DOE program managers so that the managers knew how much this really cost. The fourth reviewer disagreed with the aforementioned reviewers and asserted that the budget of \$1 million (i.e., an increase from \$450,000 in FY 2011) was excessive for this effort, even though this project had good relevance to ABR.

Section Acronyms

The following list of Acronyms cited within this section is provided as a reference for readers.

Acronym	Definition
3D	Three Dimensional
A123	A123 Systems
ABA	Anion Binding Agents
ABR	Advanced Battery Research
ABRT	Advanced Battery Research for Transportation
AC	Alternating Current
Ah	Ampere-hour
ALD	Atomic Layer Deposition
AIF3	Aluminum Fluoride
Al2O3	Aluminum Oxide
ANL	Argonne National Laboratory
ARPA-E	Advanced Research Projects Agency-Energy
ARRA	American Recovery and Reinvestment Act
B4C	Boron carbide
BASF	A chemical company
BATT	Batteries for Advanced Transportation Technologies
BDMS	Battery Database Management System
BES	DOE Basic Energy Sciences
BEV	Battery Electric Vehicle
BMS	Battery Management System
BNL	Brookhaven National Laboratory
С	Carbon
САЕВАТ	Computer-Aided Engineering of Batteries
CAFÉ	Corporate Average Fuel Economy
СВ	Carbon Black
CFF	Cell Fabrication Facility (Prototype)
СМС	Carboxymethyl Cellulose
CNT	Carbon Nanotubes
Со	Cobalt
CO2	Carbon Dioxide
CSCG	Core-Shell with Concentration Gradient
CSTR	Continually Stirred Tank Reactor
DADT	Developmental & Applied Diagnostic Testing
DBBB	2,5-di-tert-butyl-1,4-bis(2-methoxyethoxy)benzene
DC	Direct Current
DFT	Density Functional Theory
DoD	Depth of Discharge
DOE	Department of Energy

Acronym	Definition
DoE	Design of Experiment
DSC	Differential Scanning Calorimetry
EB	Electron Beam
EC	Ethylene Carbonate
EDAX	Energy Dispersive Analysis X-Ray
EIS	Electrochemical Impedance Spectroscopy
EMC	Ethyl Methyl Carbonate
EOL	End of Life
ES124	DOE Energy Storage Program (advanced prognostics modeling tool)
ESCA	Electron Spectroscopy for Chemical Analysis
ESMS	Energy Storage Monitoring System
ESR	Equivalent Series Resistance
EUCAR	European Council for Automotive R&D
EV	Electric Vehicle
EXAFS	Extended X-ray Absorption Fine Structure
FEC	Fluorinated Ethylene Carbonate
FST	Fast Summation Transformation
FTIR	Fourier Transform Infrared Spectroscopy
GHS	Greenhouse
GITT	Grid Integration Tech Team
HCSD	Harmonic Compensated Synchronous Detection
HEV	Hybrid Electric Vehicle
HEXRD	High-Energy X-Ray Diffraction
HF	Hydroflouric acid
HFiPP	Hexafluoro-iso-Propyl Phosphate
HNEI	Hawaii Natural Energy Institute
HWCVD	Hot-Wire Chemical Vapor Deposition
ICA	Interface Control Additives
IL	Ionic Liquid
IMB	Impedance Measurement Box
INL	Idaho National Laboratory
JCI	Johnson Controls, Inc.
JMI	John Marvin, Inc.
L	Liter
LBL	Lawrence Berkeley National Laboratory
LANL	Los Alamos National Laboratory
LBNL	Lawrence Berkeley National Laboratory
LCO	Lithium Cobalt Oxide (LiCoO2)
LEESS	Lower-Energy Energy Storage System
LFO	Lithium Iron Oxide
LFP	Lithium Iron Phosphate

Acronym	Definition
LG	LG Chem
LIB	Lithium-Ion Battery
LiBF4	Lithium tetrafluoroborate
LiBOB	Lithium bis(oxalato)borate
LiFOP	Lithium tetrafluorooxalatophosphate LiPF ₄ (C ₂ O ₄)
LiFSI	Lithium bis(fluorosulfonyl)imide
LiMn2O4	Lithium Manganese Oxide
LiMO2	Lithiated transition metal oxides
Li2MnO3	Lithiated transition metal oxides
LiPF6	Effective electrolyte salt for lithium-ion battery
LiTFSI	Lithium Bis(Trifluoromethanesulfonyl)Imide
LLC	Layered Lithium metal oxide Cathode
LMNO	Ni-substituted manganese spinel oxides
LMO	Lithium Manganese Oxide
LMP	Lithium Metal Polymer
LMR	Lithium Manganese Rich
LTDI	Lithium 4,5-dicyano-2-(trifluoromethyl)imidazole
LVO	Lithiated Vanadium Oxide
MAX	Layered ternary carbides, nitrides, and carbonitrides consisting of "M", "A", and "X" layers
MXene	Exfoliated MAX phases (2D structures)
МСМВ	Mesocarbon Microbeads
MD	Molecular Dynamics
MERF	Materials Engineering Research Facility (Argonne National Lab)
MIT	Massachusetts Institute of Technology
Mn	Manganese
Мо	Molybdenum
МО	Carbon and oxides (MO=SiO, SiO2, SnO2, MoO3, GeO2)
NCSU	North Carolina State University
NCA	Battery cathode material (nickel cobalt aluminum oxide)
NCM	See NMC
NETL	National Energy Technology Laboratory
NG	Natural Graphite
Ni	Nickel
NIST	National Institute of Standards and Technology
NMC	Nickel Manganese Cobalt oxide
NMP	N-Methylpyrrolidone
NMR	Nuclear Magnetic Resonance
NREL	National Renewable Energy Laboratory
NY-BEST	New York Battery and Energy Storage Technology Consortium
OCV	Open Current Voltage
OEM	Original Equipment Manufacturer

Acronym	Definition
РС	Propylene Carbonate
PEI	Polyethyleneimine
PEO	Polyethylene Oxide
PEV	Plug-in Electric Vehicle
PF6	Hexafluorophosphate
PFOP	Polyfluorene Polymer
PHEV	Plug-In Hybrid Electric Vehicle
PHEV10	Plug-In Hybrid Electric Vehicle with a 10-mile range on a single charge
PHEV40	Plug-In Hybrid Electric Vehicle with a 40-mile range on a single charge
PI	Principal Investigator
PM	Project Manager
PNNL	Pacific Northwest National Laboratory
PRIMET	Primet Precision Materials, Inc.
PS	Polystyrene
РТС	Positive Temperature Coefficient
PV	Photovoltaic
QC	Quality Control
RS2	Redox Shuttle-2
Sb	Antimony
SBR	Styrene Butadiene Rubber
SCP	Spherical Carbon Particles
SEI	Solid Electrolyte Interface
SEM	Scanning Electron Microscope
SEO	Poly(Styrene-block-Ethylene Oxide)
SES	Triblock Co-polymers (polystyrene-block-polyethylene-block-polystyrene)
Si	Silicon
SIC	Single Ion Conducting
SiO2	Silicon Oxide
Sn	Tin
SNL	Sandia National Laboratory
SOA	State of the Art
SOC	State of Charge
SOH	State of Health
SOP	Standard Operating Procedures
SSRL	Stanford Synchrotron Radiation Light Source
SUNY	State University of New York
SW	Software
тсо	Total Cost of Ownership
TEG	Thermoelectric Generator
ТЕМ	Transmission Electron Microscope
TFSI	Bis(trifluoromethane)sulfonimide [(CF3SO2)2N]

Acronym	Definition
THF	Tetrahydrofuran
Ti2C	Type of MXene (HF treated Ti2AlC)
ТМ	Transition Metal
TMS	Tetramethylsilane
TR	Time-Resolved
ТТТ	3,5-triallyl-[1,3,5]triazinane-2,4,6-trione
UHEM	Ultra-High Energy Ball Milling Machine
UHMW	Ultra-High Molecular Weight
URI	University of Rhode Island
USABC	US Advanced Battery Consortium
USC	University of Southern California
V	Volts
VC	Vinylene Carbonate
VDA	Verband der Deutschen Automobilindustrie or Association of German Automobile Manufacturers
XANES	X-ray Absorption Near Edge Spectroscopy
XAS	X-ray Absorption Spectroscopy
XPS	X-ray Photoelectron Spectroscopy
XRF	X-Ray Fluorescence
XRD	X-Ray Diffraction (Crystallography)