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RPPR Final Report
as of 21-Nov-2018

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Final Report for Period Beginning 01-Jan-2018 and Ending 30-Jun-2018

Title: Symposium EN6, Safer and More Energy-Dense Rechargeable Batteries, 2018 MRS Spring Meeting

Begin Performance Period: 01-Jan-2018

End Performance Period: 30-Jun-2018

Report Term: 0-Other

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Major Goals: Rechargeable alkali-ion batteries are the dominant form of energy storage for consumer electronics today and are increasingly finding large-scale applications such as transportation and grid storage. However, the recent spate of highly publicized lithium-ion battery fires in automotive, aviation, and consumer electronics have brought to the forefront the need to develop novel materials and battery architectures that can support higher energy densities without sacrificing safety.

The aim of Symposium EN06 is to promote a holistic approach to developing safer and more energy dense rechargeable alkali-ion batteries by providing a forum for technical, interdisciplinary discussions spanning the entire continuum from materials design to device engineering. The symposium covered novel materials discovery, characterization and fundamental understanding of safety, and cutting-edge battery architectures.

Accomplishments: The aim of Symposium EN06 of the MRS Spring 2018 meeting is to promote a holistic approach to developing safer and more energy dense rechargeable alkali-ion batteries through novel materials discovery, characterization and fundamental understanding of safety, and cutting-edge battery architectures. The symposium hosted researchers from academia, national laboratories and industry, and featured 92 presentations, including 63 oral presentations (of which 16 were invited speakers from national labs, industry, and universities from across the world) and 29 poster presentations. The four-day full day event saw a large crowd throughout the program with peak attendance well above 150 people. Fourteen invited speakers from academia were provided registration fee support to recognize their contributions to the meeting and encourage future participation. Of these, three were junior faculty (assistant professors) whose registration fees were completely covered.

Training Opportunities: Nothing to Report

Results Dissemination: The 2018 MRS Spring meeting program and abstracts may be viewed on the MRS website: www.mrs.org

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

RPPR Final Report
as of 21-Nov-2018

PARTICIPANTS:

Participant Type: Co PD/PI

Participant: Shyue Ping Ong PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co PD/PI

Participant: Jeff Sakamoto PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co PD/PI

Participant: Kang Xu PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

National Academy Member: N

Other Collaborators:

Funding Support:

Participant Type: Co PD/PI

Participant: Byoungwoo Kang PhD

Person Months Worked: 1.00

Project Contribution:

International Collaboration:

International Travel:

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Article Title: Adoption of thermal behavior as an indicator for enhancement of the EIS analysis for NCR 18650B Commercial Lithium-ion batteries system

Authors: Bo Dong, Yige Li, Kazi Ahmed, Cengiz Sinan Ozkan, Mihrimah Ozkan

Keywords: energy storage interface modeling thermodynamics

Abstract: It is of great significance to understand and monitor the condition of the commercial batteries in EVs/HEVs and stationary applications under their real working situations. Electrochemical impedance spectroscopy (EIS) has been proved to be a powerful technique for investigating the kinetics and redox reactions at the interfaces, as well as the diffusion behavior in the bulks of every electrochemical systems. Focusing on tracing the temperature of the commercial batteries during the EIS tests at different stages in a well-designed four-week driving simulation, the value of temperature profile during the EIS test as an enhanced indicator to help analyzing the formation of the passivation layers, electrolyte impedance development as well as lithium plating on the anode through EIS analysis have been found.

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Report to Army Research Office (ARO)

MRS 2018 Spring Meeting, Phoenix, AZ, Apr 2-6, 2018

Symposium EN06: Safer and More Energy-Dense Rechargeable Batteries

Shyue Ping Ong (University of California, San Diego)

Jeff Sakamoto (University of Michigan)

Kang Xu (U. S. Army Research Lab)

Byoungwoo Kang (Pohang University of Science and Technology)

Summary

The aim of Symposium EN06 of the MRS Spring 2018 meeting is to promote a holistic approach to developing safer and more energy dense rechargeable alkali-ion batteries through novel materials discovery, characterization and fundamental understanding of safety, and cutting-edge battery architectures. The symposium hosted researchers from academia, national laboratories and industry, and featured 92 presentations, including 63 oral presentations (of which 16 were invited speakers from national labs, industry, and universities from across the world) and 29 poster presentations. The four-day full day event saw a large crowd throughout the program with peak attendance well above 150 people. Fourteen invited speakers from academia were provided registration fee support to recognize their contributions to the meeting and encourage future participation. Of these, three were junior faculty (assistant professors) whose registration fees were completely covered.

Objectives

Rechargeable alkali-ion batteries are the dominant form of energy storage for consumer electronics today and are increasingly finding large-scale applications such as transportation and grid storage. However, the recent spate of highly publicized lithium-ion battery fires in automotive, aviation, and consumer electronics have brought to the forefront the need to develop novel materials and battery architectures that can support higher energy densities without sacrificing safety.

The aim of Symposium EN06 is to promote a holistic approach to developing safer and more energy dense rechargeable alkali-ion batteries by providing a forum for technical, interdisciplinary discussions spanning the entire continuum from materials design to device engineering. The symposium covered novel materials discovery, characterization and fundamental understanding of safety, and cutting-edge battery architectures.

Research Highlights

The 63 oral presentations and 29 posters were divided into several topical sessions:

EN06.01: Safe and Energy--Dense Batteries: This opening session that was comprised entirely of three invited talks from world-renowned experts was intended to provide an overview into various approaches to achieving safe and energy-dense batteries. M. Stanley Whittingham (Binghamton University) gave a talk on multi-electron intercalation reactions as a potential approach to achieving much higher capacity cathode materials. This is in contrast to current cathode technology, which mostly functions on the basis of a single electron/Li intercalation per

transition metal. Akitoshi Hayashi (Osaka Prefecture University) discussed the fabrication of positive electrode materials in all-solid-state rechargeable Li or Na batteries to achieve high capacities. He showed how formation of favorable and large contact areas between electrode and electrolyte can be achieved by electrolyte coating on electrode particles via gas-phase or liquid-phase techniques. Finally, Boris Kozinsky (Harvard University) provided an overview of modelling approaches to study Li-ion transport in amorphous solid electrolytes.

EN06.02: Electrode--Electrolyte Interfaces: Lincoln Miara (Samsung Electronics) discussed the outcomes from a computational thermodynamic study to analyze the stability between several relevant solid electrolyte-electrode interfaces. Miaofang Chi (ORNL) presented her high resolution, in situ TEM analysis of Li metal-solid electrolyte interfaces. Al Masias (University of Michigan/Ford) presented new perspectives on the mechanical properties of metallic Li at room temperature. Stack pressures used when cycling Li metal solid-state batteries are comparable to the yield strength of Li. Stefan Adam (National University of Singapore) presented his research on transition metal fluorides for as cathodes.

EN06.03: All-Solid-State Batteries: Ye Zhang (University of Houston) presented his approach for stabilizing the $\text{Na}_3\text{SbS}_4/\text{Na}$ interface by introducing a cellulose-supported poly(ethylene oxide) (CPEO) layer between Na_3SbS_4 and Na. Owing to the high stability of the CPEO layer and the enhanced interfacial contact with Na, the Na/CPEO/ Na_3SbS_4 /CPEO/Na symmetric cell shows stable Na stripping/plating behavior. Yamada Hirotohi (Nagasaki University) presented a non-intuitive result indicating that exposing garnet LLZTO powders before densification modifies the grain boundary chemistry to improve resistance to Li metal penetration. A critical current density (CCD) of 0.6 mA/cm^2 was achieved with powders intentionally exposed to air before densification.

EN06.05: Solid Electrolytes: Huanan Duan (Shanghai Jiao Tong University) presented his study on optimizing the LLZO garnet preparation process to obtained materials with good air stability and room-temperature conductivity in the range of $4\sim 6 \times 10^{-4} \text{ S cm}^{-1}$. Feng Pan (Peking University China) presented work on structures and properties of cathode materials of Li-ion batteries. Corsin Battaglia (EMPA) presented his research on $\text{Na}_2(\text{B}_{12}\text{H}_{12})_{0.5}(\text{B}_{10}\text{H}_{10})_{0.5}$, that simultaneously offers high sodium ion conductivity of 0.9 mS cm^{-1} at 20°C , excellent thermal stability up to at least 300°C , and importantly, a large electrochemical stability window of 3 V including stability versus metallic Na enabling long-term stripping and plating and the use of a sodium metal anode. Lastly, Randy Jalem (JST) conducted atomistic-level computational modelling to elucidate the effect of atomic defects that block ionic conductivity in garnet electrolyte to include Ga and protons.

EN06.06: Li--Sulfur Batteries: This session featured two invited speakers: Dr. Tim Arthur from Toyota presented their efforts in developing all-solid Li-sulfur batteries in line with Toyota's recent year investment in sulfur-based solid electrolytes. The talk was focused on in-situ characterization of the interfaces using synchrotron techniques rather than battery performances of the sulfur-Li systems. Dr. Bugga from NASA-JPL talked about the efforts of developing Li-sulfur high energy batteries for space and military applications.

EN06.07: High--Energy Cathodes: Prof. Shirley Meng from UC San Diego presented the work from her group on the frontier topic of anion-redox chemistry in transition metal oxide and the possibility of harnessing such chemistry for high capacities beyond 300 mAh/g . The atomic-resolution characterization tools developed recently via TEM and STEM techniques enabled us to peer into more details of the irreversible phase-changes near the cathode/electrolyte interfaces, which serves as guidelines to stabilize the structure. Dr. Wolverton of Northwestern University

highlighted the recent advances in developing Li-rich materials based on Fe/Mn oxides. The voltage fading caused by structural instability still presents severe challenge in harnessing these aggressive redox reactions for high capacity. Dr. Xiaolin Li from PNNL summarized their efforts in Na-ion battery materials, and concluded that interphases in the Na versions of the rechargeable batteries still remain little understood, and constitutes the key to higher energy Na-ion chemistries.

EN06.08: Devices: In this session, various speakers talked about innovative means to configure the devices. Dr. Bruce Dunn (UCLA) lectured the 3D printable electrodes and hierarchical design of battery devices based on 3D-printing technology. Prof Jung from Ulsan University presented diagnostic techniques using 3 electrode device to examine the very challenging all-solid batteries.

EN06.09: Anodes I: Yue Qi (Michigan State University) discussed recent modeling methodology developed to compliment in-situ observations in order to elucidate the underlying factors contributing to mechanistic failures. Dingchang Lin (Stanford University) presented an electrolyte-proof design of three-dimensional Li metal anode where most of the Li domains are embedded in a Li-ion conductive matrix. Chonghang Zhao (Stony Brook University) presented morphological changes and degradation of the Si nano-porous electrode during charging and discharging by using synchrotron-based X-ray nano-tomography.

EN06.10: Li Metal Anodes: M V Reddy (National University of Singapore) discussed electrochemical properties of nanocomposites of divalent transition metal oxides MO (M= Mn, Fe, Co, Ni, Cu) and LiF. Fang Liu (University of California, Los Angeles) presented the way to stabilize the interface of lithium metal anodes for advanced rechargeable batteries by using hermetic coating layer with Vapor deposition. David Mitlin (Clarkson University) discussed the advantages of selenium (Se) lithium and sodium metal cathodes that are monolithic and free-standing, and with record Se loading of 70 wt%. Gillian Hawes (University of Waterloo) presented several non-porous carbon-based thin films that can act as selectively-permeable lithium-ion membranes and as protective intermediaries between the lithium metal anode and the electrolyte.

EN06.11: Anodes II: Martin Winter (University Munster) discussed intrinsic cell safety and the prominent role of the electrolyte and how different additives influence the different components of a LIB cell and cell safety. Taehoon Kim (Okinawa Institute of Science and Technology) presented the way to obtain stable SEI formation by using a multi-layer of stacked-graphene (8-layers) grown by chemical vapor deposition (CVD). Daniel Koch (National University of Singapore) discussed the possibility of further Ti oxidation or O reduction in terms of charge density increase or depletion around the corresponding nuclei, at least in a theoretical framework. Wim Soppe (ECS-Solliance) presented a method based on Plasma Enhanced Chemical Vapor Deposition (PECVD) to create self-organized nano-structured silicon layers, which can accommodate the large volume changes and its advantages.

EN06.13: Beyond Li-Ion: Yun Jung Lee (Hanyang University) discussed the ways to achieve reversible Li-O₂ battery operations with high energies by tackling these instabilities through the synergistic integration of dual soluble catalysts for both discharging and charging with antimony tin oxide (ATO) non-carbon electrodes with a porous inverse opal structure. Hye Ryung Byon (KAIST) presented the insights into design of the carbon electrode surface toward the enhancement of discharge capacity, charge potential and cycling stability. It also paves the way for improvement of Li-O₂ cell performance in the absence of additional promoters. Di-Yan Wang (Tunghai University) talked about recent work related to development of Aluminum ion battery (AIB) and

the way to increase the cathode capacity in AIB and understanding details of the anion-graphite intercalation mechanism.

EN06.14: High Energy Density Li-Ion Electrodes: Ji-Quang Zhang (PNNL) discussed a novel “localized high concentration electrolyte (LHCE)” that enables dendrite-free cycling of lithium metal anodes with high coulombic efficiency (99.5%) and excellent capacity retention of Li metal batteries. Zhenpeng Yao (Northwestern University) presented a novel computational mechanistic approach that provides a detailed explanation of the hysteresis and non-equilibrium reaction pathways associated with typical conversion-type electrodes such as Co_3O_4 and NiO . Meng Cheng (University of Illinois at Chicago) presented the hybrid electrolyte ink that is directly printed on electrodes without any surface treatment for the substrate and post-processing for the electrolyte by using elevated-temperature DIW process. Wei Wang (Huazhong University of Science and Technology) presented developing sodium ferrous sulfate (NFS) that can have relatively high operating voltage (average discharge voltage at 3.8 V) with superior Na intercalation kinetics by using carbon coating and PC electrolyte. Junjie Niu (University of Wisconsin-Milwaukee) presented novel approach to stabilize Sn by using Skin Grafting route. Shuang Gao (University of Kentucky) presented electrochemical properties of Zr-doped NCM-811 materials.

In terms of funding management, the symposium EN06 organizers used the ARO grant to pay for registration fees for invited speakers who were carefully selected based on three criteria: (1) innovation of the work, (2) importance of the work to advances in energy storage technologies, and (3) reputation of the scientist. To promote the participation of junior faculty, full support for registration fees were provided for assistant professors, while partial support was provided for associate and full professors.

Contributions to the Discipline

Symposium EN06 brought together an interdisciplinary group of researchers and engineers, from academia, national labs and industry, focused on experimental, theoretical, and computational efforts to understand and design materials for safer and more energy-dense rechargeable batteries. The symposium has provided a forum for technical, interdisciplinary discussions spanning the entire continuum from materials design to device engineering, covering a range of topics from novel materials discovery to characterization and fundamental understanding of safety, to cutting-edge battery architectures. We believe this has generated a greater appreciation for the multi-faceted challenges in the field and promoted collaborations and cross-pollination of ideas.

More than 110 abstracts were submitted, of which 92 were selected after the critical review process mandated by MRS. It is the organizers’ firm belief that the ideas and collaborations fostered by the symposium EN06 will drive the successful design of new materials for applications in the rechargeable batteries that are not only safer, but also exhibit higher energy densities.

Future Directions

The development of safe and energy dense rechargeable batteries remains a key enabler for a sustainable energy future. The MRS has been extremely supportive of this important area of research, and we expect this trend to continue, or even accelerate, in the near future. Increasingly, researchers are finding that the critical factors to safe and high energy battery dense lies not in merely bulk materials development, but rather the holistic development of all components and the interactions between them. The development of advanced characterization and theory efforts in this regard is expected to feature heavily in future conference symposia.

Acknowledgements

We gratefully appreciate support from the Army Research Office (ARO), which was critical to the success of this symposium. We also want to thank MRS staff for supporting the application of this ARO grant.

SYMPOSIUM EN06

Safer and More Energy-Dense Rechargeable Batteries
April 3 - April 6, 2018

Symposium Organizers

Byoungwoo Kang, POSTECH
Shyue Ping Ong, University of California, San Diego
Jeff Sakamoto, University of Michigan
Kang Xu, U.S. Army Research Laboratory

Symposium Support Army Research Office

MRS Invitation to Publish

All authors are invited to submit articles based on their 2018 MRS Spring Meeting presentations to journals in the MRS portfolio. (www.mrs.org/publications-news) Papers submitted and accepted for publication in MRS Advances (www.mrs.org/mrs-advances) will be available as symposium collections. Visit the MRS/Cambridge University Press Publications Booth #100 in the Exhibit Hall to learn more, including MRS Advances print options available at special rates during the meeting week only.

* Invited Paper

SESSION EN06.01: Safe and Energy-Dense Batteries
Session Chairs: Shyue Ping Ong and Jeff Sakamoto
Tuesday Morning, April 3, 2018
PCC North, 100 Level, Room 121 B

10:30 AM *EN06.01.01

Can Multi-Electron Intercalation Reactions be the Basis of THE Next Generation Batteries? M. Stanley Whittingham; State University of New York at Binghamton, United States.

11:00 AM *EN06.01.02

Design of Positive Electrode Layers for All-Solid-State Rechargeable Batteries with High Energy Density Akitoshi Hayashi; Osaka Prefecture University, Japan.

11:30 AM *EN06.01.03

Li-Ion Transport Modeling in Amorphous Solid Electrolytes Boris Kozinsky^{1,2}; ¹Robert Bosch LLC, United States; ²Harvard University, United States.

SESSION EN06.02: Electrode-Electrolyte Interfaces
Session Chairs: Shyue Ping Ong and M. Stanley Whittingham
Tuesday Afternoon, April 3, 2018
PCC North, 100 Level, Room 121 B

1:30 PM *EN06.02.01

Unlocking High Voltage Stability in all Solid State Batteries Lincoln Miara; Samsung Electronics, United States.

2:00 PM *EN06.02.02

Formation and Stability of Solid Electrolyte-Electrode Interfaces Probed by Electron Microscopy Miaofang Chi; Oak Ridge National Laboratory, United States.

2:30 PM BREAK

3:30 PM *EN06.02.03

Mechanical Properties of Lithium—Past, Present and Future Alvaro Masias^{1,2}; ¹Ford Motor Company, United States; ²University of Michigan, United States.

4:00 PM *EN06.02.04

Design of Materials for Safe High Rate Capability Batteries Stefan N. Adams; National University of Singapore, Singapore.

SESSION EN06.03: All-Solid-State Batteries
Session Chairs: Miaofang Chi and Lincoln Miara
Tuesday Afternoon, April 3, 2018
PCC North, 100 Level, Room 121 B

4:30 PM EN06.03.01

Enhancing Interfacial Stability Between the Solid Electrolyte and Sodium Metal Anode via Polymer Interlayer Ye Zhang; University of Houston, United States.

4:45 PM EN06.03.02

Modification of Grain-Boundary to Suppress Lithium Growth Through Garnet-Type Solid Electrolyte Hirotsushi Yamada; Nagasaki Univ, Japan.

SESSION EN06.04: Poster Session I

Tuesday Afternoon, April 3, 2018
5:00 PM - 7:00 PM
PCC North, 300 Level, Exhibit Hall C-E

EN06.04.01

High Capacity All-Solid-State Sodium Metal Battery with Hybrid Polymer Electrolyte Yongwei Zheng; Drexel University, United States.

EN06.04.02

Ion Beam Irradiated Graphenic Layers as Lithium Ion Battery Anodes Prateek Hundekar; Rensselaer Polytechnic Institute, United States.

EN06.04.03

Polymer-Assisted Deposition Li(Ni,Co,Mn)O₂ Thin Films Di Huang; New Mexico State University, United States.

EN06.04.04

Atomic-Scale Control of Silicon Expansion Space as Ultrastable Battery Anodes Jian Zhu; Hunan University, China.

EN06.04.05

The Studies of Lattice Parameter and Electrochemical Behavior for Li₃V₂(PO₄)₃/C Cathode Materials Min-Young Kim; Korea Institute of Industrial Technology, Korea (the Republic of).

EN06.04.06

Observation of Interfacial Dynamics in Magnesium Batteries Using Operando XAS/TEM Khim Karki; Hummingbird Scientific, United States.

EN06.04.07

High-Power Alternative-Ion Batteries via Co-Intercalation Jennifer Donohue^{1,2}; ¹State University of New York at Binghamton, United States; ²Vanderbilt University, United States.

EN06.04.08

Modification of LiFePO₄ Cathode with 3D “Silk flowers” Like Ni-Al-Li-LDHs in Lithium-Ion Battery Xiaoqing Zhang; University of Electronic Science and Technology of China, China.

EN06.04.09

The Effect of Calendering Temperature for Sulfur Electrodes Used for Large-Scale Lithium-Ion Batteries Rachel Ye; University of California, Riverside, United States.

EN06.04.10

Novel High Sulfur Loading Cathodes for High Performance Li-S Batteries Ji Hoon Kang; KOREATECH, Korea (the Republic of).

EN06.04.11

Lithium-Sulfur Batteries—Effect of Electrolyte and Sulfur Loading on the Electrochemical Performance Ji Hoon Kang; KOREATECH, Korea (the Republic of).

EN06.04.12

A New Design Concept of Li-S Battery Based on the Reaction Mechanism of Sulfur for High Performance Energy Storage Systems Jin Kyeong Kang; KOREATECH, Korea (the Republic of).

EN06.04.13

A Highly Robust Sulfur Cathode with a Structure Stabilizer for a Long-Life Li-S Battery Jong Won Park; KOREATECH, Korea (the Republic of).

EN06.04.14

Inverse Vulcanization with Functional Linkers—Towards New Cathode Active Materials Hancol Kang; POSTECH, Korea (the Republic of).

EN06.04.15

Highly Stable 3D Nanoporous SnSb Alloy as a Lithium Storage Material
Yoon Yun Lee; Yonsei University, Korea (the Republic of).

EN06.04.16

Synthesis and Electrochemical Performance of Sn-Fe Alloy with High and Stable Capacity as Anodes in Lithium-Ion Batteries Fengxia Xin; Binghamton University, United States.

EN06.04.17

Inert Gas Annealing of $\text{Li}_4\text{T}_2\text{O}_{12}$ Targeting Improvement of Conductivity
Joe Sakai; University of Tours, France.

EN06.04.18

Effects of Porous Media Selection in Lithium Iron Phosphate Cathodes
Jeffrey Geiger^{1,2}; ¹University of California, Riverside, United States; ²University of California, Riverside, United States.

EN06.04.19

Scalable Synthesis of High Capacity and High Cyclability Polyethylene Terephthalate (PET)-Derived Graphite Anode for Lithium-Ion Battery
Taner Zerrin; University of California, Riverside, United States.

EN06.04.20

Thermal Stability Analysis of Lithium-Sulfur Batteries via Controlled Conditioning Techniques Daisy Patino; University of California, Riverside, United States.

EN06.04.21

An Analysis of Lithium Sulfur Interactions via GITT Measurements
Daisy Patino; University of California, Riverside, United States.

EN06.04.22

The Effects of Electrode Density on Sulfur and Silicon Performance for Lithium-Ion Batteries Jeffrey M. Bell; University of California, Riverside, United States.

EN06.04.23

Electrochemical Analysis of Bismuth Nanotubes and WS₂ Electrode Materials Imbedded in Flexible Perchlorate-Based Polymer Gel Electrolyte for Use in Mg-Ion Battery Cells Todd K. Houghton; Arizona State University, United States.

EN06.04.24

Improving Performance of LFP Cathodes by Optimizing Porosity
Jiyong Kim; University of California, Riverside, United States.

EN06.04.25

Sodium Storage in Rippled Bilayer Graphene—A Model for Amorphous Carbon Anodes Weiyi Zhang; University of California, Riverside, United States.

EN06.04.26

Synthesis of LiFePO_4 in a Limited Air Environment—Synthesis Time Study and Optimization Fei Gu^{1,2}; ¹University of California, Riverside, United States; ²Winston Chung Global Energy Center, University of California, Riverside, United States.

EN06.04.27

Scalable Silicon-Carbon Nanospheres Electrodes for Lithium-Ion Batteries
Jingjing Liu; University of California, Riverside, United States.

EN06.04.28

Stability and Electrochemical Performance of Different LiVOPO_4 Phases
Marc Francis V. Hidalgo; Binghamton University, United States.

EN06.04.29

A First-Principles Investigation of Lithium Intercalation and Diffusion in Titanium Dioxide with Oxygen Vacancy Hsiu-Liang Yeh; National Central University, Taiwan.

SESSION EN06.05: Solid Electrolytes

Session Chairs: Timothy Arthur and Ratnakumar Bugga
Wednesday Morning, April 4, 2018
PCC North, 100 Level, Room 121 B

8:00 AM *EN06.05.01

Synthesis, Air Stability and Applications of $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Huanan Duan; Shanghai Jiao Tong University, China.

8:30 AM *EN06.05.02

Structures and Properties of Cathode Materials of Li-Ion Batteries
Feng Pan; Peking University, China.

9:00 AM *EN06.05.03

A Stable 3 V All-Solid-State Sodium-Ion Battery Based on a Closo-Borate Electrolyte Corsin Battaglia; Empa-Swiss Federal Laboratories for Materials Science and Technology, Switzerland.

9:30 AM BREAK

10:00 AM EN06.05.04

Computational Investigation on Oxide Electrolytes with Garnet Structure and Conduction-Pathway-Blocking Dopants Randy Jalem^{1,2}; ¹Japan Science and Technology Agency (JST), PRESTO, Japan; ²National Institute for Materials Science – Global Research Center for Environment and Energy based on Nanomaterials Science (NIMS-GREEN), Japan.

SESSION EN06.06: Li-Sulfur Batteries

Session Chairs: Y. Shirley Meng and Christopher Wolverton
Wednesday Morning, April 4, 2018
PCC North, 100 Level, Room 121 B

10:15 AM *EN06.06.01

All- Solid Lithium- Sulfur Batteries Timothy S. Arthur; Toyota Research Institute, United States.

10:45 AM *EN06.06.02

High Energy Density Lithium/Sulfur Batteries for NASA and DoD Applications Ratnakumar Bugga; U.S. Army RDECOM CERDEC, United States.

11:15 AM EN06.06.03

An Alternative to Prelithiation for Full Cells Utilizing Sulfur Cathodes
Rachel Ye; University of California, Riverside, United States.

11:30 AM EN06.06.05

Ultrathin and Lightweight Interlayers Based on Carbon Nanotube Film and Metal Oxides/Sulfides/Phosphides as Efficient Polysulfide-Trapping Shields for Li-S Batteries Jiaping Wang; Tsinghua University, China.

SESSION EN06.07: High-Energy Cathodes

Session Chairs: Xiangfeng Duan and Jeff Sakamoto
Wednesday Afternoon, April 4, 2018
PCC North, 100 Level, Room 121 B

1:30 PM *EN06.07.01

From Cation Redox to Anion Redox Electrochemistry Y. Shirley Meng^{1,2}; ¹University of California, San Diego, United States; ²Sustainable Power and Energy Center, United States.

2:00 PM *EN06.07.02

Materials Design of High-Energy Cation/Anion Redox in Li-Rich Cathode Materials— Li_3FeO_4 , $\text{Li}_4\text{Mn}_2\text{O}_5$ and Li_2MO_3 Christopher Wolverton; Northwestern University, United States.

2:30 PM BREAK

3:30 PM *EN06.07.03

Towards High Energy Na-Ion Batteries Xiaolin Li; Pacific Northwest National Laboratory, United States.

4:00 PM EN06.07.04

Obstacles Toward Unity Efficiency of $\text{LiNi}_{1-2x}\text{Co}_x\text{Mn}_x\text{O}_2$ ($x=0\sim 1/3$) (NCM) Cathode Materials—Insights from *Ab Initio* Calculations
Chaoping Liang^{1,2}; ¹State Key Laboratory of Powder Metallurgy, Central South University, China; ²The University of Texas at Dallas, United States.

4:15 PM EN06.07.05

Atomic Thermal Migration Studies on Layered Cathode Materials for Li-Ion Batteries by Using *In Situ* High Temperature Neutron Diffraction and Gas Analyses Hyungsub Kim; Korea Atomic Energy Research Institute (KAERI), Korea (the Republic of).

4:30 PM EN06.07.06

Electrophoretic Deposition as a Manufacturing Strategy for High Areal Capacity Cathodes Kathleen Moyer; Vanderbilt University, United States.

4:45 PM EN06.07.07

Synthesis and Characterization of Li Excess Mo-Based Cathodes for Li-Ion Batteries Ethan C. Self; Oak Ridge National Laboratory, United States.

SESSION EN06.08: Devices
Session Chairs: Chunmei Ban and Yue Qi
Thursday Morning, April 5, 2018
PCC North, 100 Level, Room 121 B

8:00 AM *EN06.08.01

Photo-Patternable Lithium-Ion Electrolytes [Bruce S. Dunn](#); University of California, Los Angeles, United States.

8:30 AM *EN06.08.02

Diagnosis of All-Solid-State Batteries Using Three-Electrode Cells
[Yoon Seok Jung](#); Ulsan National Institute of Science and Technology (UNIST), Korea (the Republic of).

9:00 AM EN06.08.03

Multiscale Thermomechanical Model to Predict Thermal Runaway in Lithium-Ion Batteries [Abhishek Sarkar](#); Iowa State University, United States.

9:15 AM EN06.08.04

High Volumetric and Areal Capacity 3D-Structured Electroplated Tin Electrode [Pengcheng Sun](#); University of Illinois at Urbana-Champaign, United States.

9:30 AM EN06.08.05

High Rate and Stable Cycling of High Energy Cathode LiVOPO_4 with Nanosizing, Carbon Coating and Structure Reconstruction by a Mechanical-Thermal Method [Yong Shi](#); Binghamton University, United States.

9:45 AM EN06.08.06

Design and Synthesis of a Novel High Energy Density $\text{Li}_2\text{MnCo}_{1-x}\text{SiO}_4$ Cathode Material [Xianhui Zhang](#); NInbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, China.

10:00 AM BREAK

SESSION EN06.09: Anodes I
Session Chairs: Bruce Dunn and Yoon Seok Jung
Thursday Morning, April 5, 2018
PCC North, 100 Level, Room 121 B

10:30 AM *EN06.09.01

Effect of Surface Modification on Surface Chemistry and Electrochemistry of Silicon-Based Anode Materials [Chunmei Ban](#); National Renewable Energy Laboratory, United States.

11:00 AM *EN06.09.02

Quantify the Irreversible Structural and Chemical Changes in Nanostructured Si and SiO Electrodes [Yue Qi](#); Michigan State University, United States.

11:30 AM EN06.09.03

Stable Three-Dimensional Composite Lithium Metal Anode with Electrolyte-Proof Architecture for High-Energy and High-Power Applications [Dingchang Lin](#); Stanford University, United States.

11:45 AM EN06.09.04

Silicon Anode Morphological Evolution with Lithiation and De-Lithiation [Chonghang Zhao](#); Stony Brook University, United States.

SESSION EN06.10: Li Metal Anodes
Session Chairs: Chunmei Ban and Martin Winter
Thursday Afternoon, April 5, 2018
PCC North, 100 Level, Room 121 B

1:30 PM EN06.10.01

Synthesis and Electrochemical Studies of Metal Fluorides and Nanocomposite Metal Oxides-LiF Materials [M V Reddy](#); National University of Singapore, Singapore.

1:45 PM EN06.10.02

Hermetic Coating Layer for Lithium Metal Anode Through Vapor Deposition [Fang Liu](#); University of California, Los Angeles, United States.

2:00 PM EN06.10.03

Selenium Impregnated Monolithic Carbons as Free-Standing Cathodes for High Volumetric Energy Lithium and Sodium Metal Batteries [David Mitlin](#); Clarkson University, United States.

2:15 PM EN06.10.04

Impervious Carbon Nanomaterial Thin Films for Lithium Metal Anode Protection [Gillian Hawes](#); University of Waterloo, Canada.

2:30 PM BREAK

3:30 PM EN06.10.05

Water-Tolerant Lithium Metal Cycling Promoted via Artificial SEI Transplantation [Nikhilendra Singh](#); Toyota, United States.

SESSION EN06.11: Anodes II
Session Chairs: Yoon Seok Jung and Yue Qi
Thursday Afternoon, April 5, 2018
PCC North, 100 Level, Room 121 B

3:45 PM *EN06.11.01

Intrinsic Safety of Lithium Ion Batteries [Martin Winter](#); Universität Münster, Germany.

4:15 PM EN06.11.02

Stacked-Graphene Layers as Engineered Solid-Electrolyte Interphase (SEI) Grown by Chemical Vapour Deposition for Lithium-Ion Batteries [Taehoon Kim](#); Okinawa Institute of Science and Technology, Japan.

4:30 PM EN06.11.03

The Mismatch Between Charge and Formal Oxidation State of Titanium in Titanium Dioxide and Its Implications Towards Our View of Redox Processes [Daniel Koch](#); National University of Singapore, Singapore.

4:45 PM EN06.11.04

Self-Organized Nano-Structured Silicon as Anode Material for Li-Ion Batteries [Wim Soppe](#)^{1,2}; ¹ECN - Solliance, Netherlands; ²LeydenJar Technologies, Netherlands.

SESSION EN06.12: Poster Session II
Thursday Afternoon, April 5, 2018
5:00 PM - 7:00 PM
PCC North, 300 Level, Exhibit Hall C-E

EN06.12.01

Effect of CeLa Microalloying on the Microstructures and Mechanical Properties of Al-Cu-Mn-Mg-Fe Lithium Battery Shell Alloy [Dongyan Ding](#); Shanghai Jiao Tong University, China.

EN06.12.03

Flexible All-Solid-State Li-Te Safe Batteries [Mingqiang Zhu](#); Huazhong University of Science & Technology, China.

EN06.12.04

Toward a Dendrite Free, Powder Compact-Based Solid Electrolyte Lithium Metal Battery—Interfacial Modification [Ran Zhao](#); Iowa State University, United States.

EN06.12.05

In Situ Fabricated Carbon-Polyimide Hybrid Film Providing Mechanical and Electrical Robust Network for LIB Silicon Anode [Goojin Jeong](#); Korea Electronics Technology Institute, Korea (the Republic of).

EN06.12.06

Characterization and Electrochemical Analysis of a Novel Alkoxide-Based Electrolyte for Mg-Ion Batteries [Anushka Dasgupta](#); Princeton University, United States.

EN06.12.07

Using Thermal Behavior as an Indicator to Enhance the EIS Analysis for Lithium-Ion Battery System [Bo Dong](#); University of California, Riverside, United States.

EN06.12.08

High Energy Density, Thin and Flexible Printed Metal Air Batteries for Flexible Electronics [Taichong Ma](#); University of Washington, United States.

SESSION EN06.13: Beyond Li-Ion
Session Chairs: Byoungwoo Kang and Feng Pan
Friday Morning, April 6, 2018
PCC North, 100 Level, Room 121 B

9:00 AM *EN06.13.01

Synergistic Integration of Soluble Catalysts with Carbon-Free Electrodes for Li-O_2 Batteries [Yun Jung Lee](#); Hanyang University, Korea (the Republic of).

9:30 AM *EN06.13.02

Towards Controlling of Li_2O_2 Structures for Improvement of Charging Overpotential in Lithium-Oxygen Batteries [Hye Ryung Byon](#); KAIST, Korea (the Republic of).

10:00 AM BREAK

10:30 AM EN06.13.03

In Silico Materials Design for Next Generation Batteries [Nikhil Medhekar](#); Monash University, Australia.

10:45 AM EN06.13.04

The Role of Solid Electrolyte Interphase (SEI) at Sodium Metal Electrode for Sodium-Oxygen (Na-O₂) Batteries [Younguk Jung](#)^{1,2}; ¹Korea Advanced Institute of Science and Technology (KAIST), Korea (the Republic of); ²KAIST Institute NanoCentury, Korea (the Republic of).

11:00 AM EN06.13.05

A 3 V Stable *closo*-borate Electrolyte for All-Solid-State Sodium-Ion Batteries [Leo Duchene](#)^{1,2}; ¹Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland; ²University of Geneva, Switzerland.

11:15 AM EN06.13.06

Mechanism Studies of Anion Intercalating into Graphite Layer in Aluminum Ion Battery [Di-Yan Wang](#); Tunghai University, Taiwan.

11:30 AM EN06.13.07

Mechanically Reinforced Composite Polymer Electrolyte with High Ionic Conductivity and High Modulus Enabled by a Strong Mesoporous Backbone [Dingchang Lin](#); Stanford University, United States.

SESSION EN06.14: High Energy Density Li-Ion Electrodes
Session Chairs: Yun Jung Lee and Feng Pan
Friday Afternoon, April 6, 2018
PCC North, 100 Level, Room 121 B

1:30 PM *EN06.14.01

Highly Stable Lithium Metal Batteries Enabled by Localized High Concentration Electrolytes [Ji-Guang Zhang](#); Pacific Northwest National Laboratory, United States.

2:00 PM EN06.14.02

Revealing the Conversion Mechanism of Transition Metal Oxide/Sulfide Electrodes During the Electrochemical Lithiation [Zhenpeng Yao](#); Northwestern University, United States.

2:15 PM EN06.14.03

Exploring the Combined Anionic and Cationic Redox Reactivity in the Super Li-Rich Li₂FeO₄ Based High-Energy-Density Cathode Materials [Zhenpeng Yao](#); Northwestern University, United States.

2:30 PM EN06.14.04

Elevated-Temperature Direct Ink Writing of Hybrid Solid-State Electrolyte for 3D Printing of Li-Ion Battery [Meng Cheng](#); University of Illinois at Chicago, United States.

2:45 PM BREAK

3:15 PM EN06.14.05

A Comparative Study of the Charge Compensation Mechanism of Li_{1.3}Ni_{0.3}Ta_{0.4}O₂ and Li_{1.3}Mn_{0.4}Ta_{0.3}O₂ Disordered Rocksalt as Cathode Material for Li-Ion Battery [Quentin Jacquet](#)^{1,2,3}; ¹College de France, France; ²Université Pierre et Marie Curie, France; ³RS2E, Réseau sur le stockage électrochimique de l'énergie, France.

3:30 PM EN06.14.06

A Fe-Based Cathode Material with High Operating Voltage for Sodium-Ion Battery [Wei Wang](#); Huazhong University of Science and Technology, China.

3:45 PM EN06.14.07

Sn Wears Super Skin—A New Design for Long Cycling and High Rate Batteries [Junjie Niu](#); Univ of Wisconsin-Milwaukee, United States.

4:00 PM EN06.14.08

DFT-Guided Exploration and Experimental Testing of Dopants for Li₂FeSiO₄ High Capacity Cathode Materials [Yan Zeng](#); McGill University, Canada.

4:15 PM EN06.14.09

Zirconium-Doped Layered LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂ as A High-Rate and Durable Lithium-Ion Battery Positive Electrode Material [Shuang Gao](#); University of Kentucky, United States.

SYMPOSIUM EN07

Issues, Challenges and Opportunities in Actinide Materials
April 3 - April 5, 2018

Symposium Organizers

M. Lee Davisson, Lawrence Livermore National Laboratory
Kristina Kvashnina, European Synchrotron Radiation Facility
Jeremy Mitchell, Los Alamos National Laboratory
JG Tobin, University of Wisconsin-Oshkosh

Symposium Support

Lawrence Livermore National Laboratory
Los Alamos National Laboratory

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* Invited Paper

SESSION EN07.01: Actinide Biology, Medicine, Decontamination and Nanoscience

Session Chairs: Ladislav Havela and David Shuh
Tuesday Morning, April 3, 2018
PCC North, 100 Level, Room 126 C

10:30 AM *EN07.01.01

Exploring Trends in Bonding from Actinium to Einsteinium Using Biologically Relevant Ligands—Where Separation, Decontamination and Nuclear Medicine Meet [Rebecca Abergel](#); Lawrence Berkeley National Lab, United States.

11:00 AM *EN07.01.02

What Can Actinides Do for Metal-Organic Frameworks and What Can Metal-Organic Frameworks Do for Actinides and Fission Products? [Shuao Wang](#); Soochow University, China.

11:30 AM *EN07.01.03

Production of Ac-225 from High Energy Proton Irradiation of Thorium [C.S. Cutler](#); Brookhaven National Laboratory, United States.

SESSION EN07.02: Plutonium and Its Properties

Session Chairs: Borje Johansson, Jeremy Mitchell and Per Soderlind
Tuesday Afternoon, April 3, 2018
PCC North, 100 Level, Room 126 C

1:30 PM *EN07.02.01

A Review of the Electronic Structure of Plutonium [Gerard H. Lander](#)^{1,2}; ¹European Commission Joint Research Centre, Germany; ²Institut Laue-Langevin, France.

2:00 PM EN07.02.02

Physical Mechanism of the δ - δ' - ϵ Phase Stability in Plutonium Metal [Borje S. Johansson](#); Materials Theory, Uppsala University, Sweden.

2:15 PM EN07.02.03

Assessing Density-Functional Theory for Equation-of-State from Light Solids to Actinides [Per Soderlind](#); Lawrence Livermore National Lab, United States.

2:30 PM BREAK