



Denver Marriott West Golden, Colorado June 25-27, 2019

Hosted by

INREL

Transforming ENERGY

Contents

Welcome Letter	5
Thank You to Our Program Sponsors	5
Agenda	6
Keynote Speakers	10
Martin Keller, Ph.D.	10
Vincent L. Sprenkle, Ph.D.	11
George W. Crabtree, Ph.D.	10
Speaker Biographies	12
Session 1	12
Prashant Kumta, Ph.D.	12
Jim Zheng, Ph.D.	12
Amin Salehi-Khojin Ph.D.	12
Xiaolin Li, Ph.D.	13
Session 2	13
Kang Xu, Ph.D.	13
Seung-Tae Hong, Ph.D.	13
Kevin Zavadil	14
Session 3	14
Jason Zhang, Ph.D.	14
Nitash Balsara, Ph.D.	14
Jeff Sakamoto, Ph.D.	15
Andrew Westover, Ph.D. and Nancy Dudney, Ph.D.	15
Mike Zimmerman, Ph.D.	16
Marca Doeff, Ph.D.	16
Nick Wu, Ph.D.	16
Session 4	17
Donald R. Sadoway, Ph.D.	17
Jagjit Nanda, Ph.D.	17
Zheng Li, Ph.D.	17
Session 5	18
Evan Reed, Ph.D.	18
Alec Talin, Ph.D.	18
Kevin Roche	18
Bert de Jong, Ph.D.	19
Session 6	19
Jordi Cabana, Ph.D.	19
Maxwell Giammona, Ph.D.	19
Fulya Dogan, Ph.D.	20
Miaofang Chi, Ph.D.	20

Session 7	20
Bryant Polzin	20
Joon Kim, Ph.D.	21
Shriram Santhanagopalan, Ph.D.	21
Luis Diaz Aldana, Ph.D.	21
Speaker Abstracts	22
Session 1	23
Novel Engineering Approaches to High Energy Density Lithium Metal Batteries	23
Investigate the Formation of Discharge Products to the Limitation of Energy Density in Cathode of Li-S Batteries	23
Insights into New Li-O2 Electrochemistry Strategies for Energy Storage	24
Development of High-Performance Na-Ion Battery Cathodes	24
Session 2	25
Beyond Li-Ion Chemistries in Aqueous Electrolytes	25
Intercalation Chemistry of Mg and Ca Ions Into Host Materials for Post Li-Ion Batteries	25
Multivalent Anode Interphases: Opportunities to Direct Interfacial Cation Transport	26
Session 3	26
Non-Flammable Electrolytes for Lithium Metal Batteries	26
Predicting the Performance of Lithium Metal Electrodes Stabilized by Polymer Electrolytes	26
Electrochemical, Quantum Mechanical, and Physical Behavior of the Li Metal-Solid Electrolyte Interface	27
Can Glassy Electrolytes Enable All-Solid-State Li Metal Batteries?	27
Enabling Solid-state Batteries with Breakthrough Polymer Technology	28
Towards Solid-state Batteries with LLZO	28
Ceramic-Polymer Composite Electrolytes for Lithium-Metal Batteries Session 4	28
	29
Liquid Metal/Molten Salt Batteries for Stationary Storage	29
Enabling Redox Flow Battery Chemistries for Long Duration Energy Storage: Challenges and Opportunities Sodium-Sulfur Flow Batteries for Low-Cost Stationary Energy Storage	29 30
, 3, 3	
Session 5	30
Identification of 11 New Solid Lithium-Ion Conductors with Promise for Batteries Using Data Science Approaches	
Neuromorphic Computing with the Redox Transistor	31
Fundamentals of Quantum Computing: An Introduction for Engineers and Scientists	31
Quantum Computing as a Platform for Scientific Discovery in Chemical Sciences	32
Session 6	32
Measuring and Defining Electrochemical Reactions of Transition Metal Oxides In Mg Electrolytes	32
In-Situ Electrochemical Atomic Force Microscopy: A Powerful Tool for Understanding Metal-Air Batteries	32
Solid-state NMR Applications on Rechargeable Battery Chemistries	33 33
Understanding Conductivity and Stability of Interfaces in All Solid-State Batteries via STEM	
Session 7	34
The ReCell Center: DOE's Advanced Battery Recycling Program	34
Manufacturing with Recycling Materials	34
Quality Assessment for Used Batteries Electro-Assisted Recycling of Lithium-Ion Batteries	35 35
Licetto Assisted necycling of Ethilum for Datteries	55



Welcome Letter



Symposium on the Future of Energy Storage Beyond Lithium Ion XII

June 25-27, 2019 Golden, Colorado

Welcome to the Beyond Lithium Ion Symposium on the Future of Energy Storage at the Denver Marriott West in Golden, Colorado. This is the 12th symposium on energy storage organized by the consortium of IBM Research,

United States National Laboratories, including National Renewable, Argonne, Lawrence Berkeley, Pacific Northwest, and Oak Ridge, and the NASA Glenn Research Center to bring together industry, university, and federal scientists and engineers focused on transformational advances and the further breakthroughs needed in scalable energy storage.

Thanks to the vision of the Program Committee, this year's symposium is focused on the future of energy storage technologies for transportation and the electricity grid. Symposium themes will focus on key areas of innovation including:

- 1. Reviewing groundbreaking technical progress
- 2. Exploring future directions
- 3. Understanding critical challenges that are impeding progress.

Leading researchers and technical experts from around the world will discuss necessary materials, diagnostics, scaling, and manufacturing issues associated with better-performing energy storage devices. Through this open format dialogue, organizers aim to accelerate innovation, reduce costs, and improve the safety of advanced, electrochemical energy storage concepts and systems "beyond lithium ion."

A sincere thank you to our sponsors, whose participation and financial support is essential to the success of this event. Thank you to all the experts we will hear from over the next three days and once again, welcome to Golden, Colorado. We hope you enjoy yourself and explore all that we have to offer.

Sincerely,

Ahmad Pesaran

Ahmad A. Pesaran

General Chair, Beyond Lithium Ion XII

Thank You to Our Program Sponsors

Silver

Mercedes-Benz

Research & Development North America, Inc.

Bronze













Corporate Sponsors







Agenda

Day 1 — June 25, 2019

7:30 AM Registration | Breakfast8:30 AM Welcome (10 mins)8:40 AM Executive Welcome

Keynote

9:00 AM Transforming Energy through Innovation

Martin Keller, National Renewable Energy Laboratory

Session I: New Frontiers of Alkali Metal Batteries (Chair: Wu Xu)

9:40 AM Novel Engineering Approaches to High Energy Density Lithium Metal Batteries

Prashant Kumta, University of Pittsburgh

10:10 AM Investigate the Formation of Discharge Products to the Limitation of Energy Density in Cathode of Li-S Batteries

Jim Zheng, Florida State University

10:40 AM Break (30 mins)

11:10 AM Li-O2 Batteries: Challenges and Recent Progress

Amin Salehi-Khojin, University of Illinois at Chicago

11:40 AM Development of High-Performance Na-ion Battery Cathodes

Xiaolin Li, Pacific Northwest National Laboratory

12:10 PM Lunch

Session II: Emerging Opportunities for Multivalent Metal Anodes (Chair: Lei Cheng)

1:30 PM Beyond Li-ion Chemistries in Aqueous Electrolytes

Kang Xu, ARL

2:00 PM Intercalation Chemistry of Mg and Ca lons into Host Materials for Post Li-ion Batteries

Prof. Seung-Tae Hong, Daegu Gyeongbuk Institute of Science and Technology

2:30 PM Multivalent Anode Interphases: Opportunities to Direct Interfacial Cation Transport

Kevin Zavadil, Sandia National Laboratories

3:00 PM Break (30 mins)

Session III: Safe Electrolytes for Beyond Lithium Ion (Chair: Ray Bair and Wu Xu)

3:30 PM Non-Flammable Electrolytes for Lithium Metal Batteries

Jason Zhang, Pacific Northwest National Laboratory

4:00 PM Predicting the Performance of Lithium Metal Electrodes Stabilized by Polymer Electrolytes

Nitash Balsara, University of California Berkeley

4:30 PM Electrochemical, Quantum Mechanical, and Physical Behavior of the Li Metal-Solid Electrolyte Interface

Jeff Sakamoto, University of Michigan

5:00 PM Can Glassy Electrolytes Enable All-Solid-State Li Metal Batteries?

Andrew Westover and Nancy Dudney, Oak Ridge National Laboratory

5:30 PM Adjourn

Day 2 — June 26, 2019

7:00 AM Registration | Breakfast

Keynote

8:00 AM Energy Storage for Improved Grid Resilience and Renewables Integration

Vincent Sprenkle, Pacific Northwest National Laboratory

Session III (cont'd): Safe Electrolytes for BLI (Chair: Ray Bair and Wu Xu)

9:00 AM	Enabling Solid-State Batteries with Breakthrough Polymer Technology	av

Mike Zimmerman, Tufts University

9:30 AM Towards Solid-State Batteries with LLZO

Marca Doeff, Berkeley Lab

10:00 AM Ceramic-Polymer Composite Electrolytes for Lithium-Metal Batteries

Nick Wu, West Virginia University

10: 30 AM Break (30 mins)

Session IV: Chemistry for Electrochemical Stationary Energy Storage (Chair: Young-Hye Na)

11:00 AM	Liquid Metal/Molten Salt Batteries for Stationary Storage	
----------	---	--

Donald R. Sadoway, Massachusetts Institute of Technology

11:30 AM Enabling Redox Flow Battery Chemistries For Long Duration Energy Storage: Challenges and Opportunities

Jagjit Nanda, Oak Ridge National Laboratory

12:00 PM Sodium-Sulfur Flow Batteries for Low-Cost Stationary Energy Storage

Zheng Li, Virginia Tech

12:30 PM Lunch (1 hour)

Session V: New Frontiers of Energy Storage: Artificial intelligence, Machine Learning and Quantum Computing (Chair: Winfried Wilcke)

1:30 PM	Identification of 11	New Solid Lithium-ion	Conductors with F	Promise for Batteries	Using Data Science

Approaches

Evan Reed, Stanford University

2:00 PM Neuromorphic Computing with the Redox Transistor

Alec Talin, Sandia National Laboratories

2:30 PM Fundamentals of Quantum Computing: An Introduction for Engineers and Scientists

Kevin Roche, IBM Almaden

3:00 PM Quantum Computing as a Platform for Scientific Discovery in Chemical Sciences

Bert de Jong, Lawrence Berkeley National Laboratory

3:30 PM Break (30 mins)

Day 2 continued on next page.

Agenda

Day 2 (cont'd.) — June 26, 2019

Session VI: Advanced Characterization for Beyond Lithium-ion Technologies (Chair: Chunmei Ban)

4:00 PM	Measuring and Defining Electrochemical Reactions of Transition Metal Oxides in Mg Electrolytes Jordi Cabana, University of Illinois at Chicago
4:30 PM	In-Situ Electrochemical Atomic Force Microscopy: A Powerful Tool for Understanding Metal-Air Batteries Maxwell Giammona, IBM Almaden
5:00 PM	Solid-State NMR Applications on Rechargeable Battery Chemistries Fulya Dogan, Argonne National Laboratory
5:30 PM	Understanding Conductivity and Stability of Interfaces In All Solid-State Batteries via STEM Miaofang Chi, Oak Ridge National Laboratory
6:00- 8:30PM	Poster Session and Reception



Day 3 — June 27, 2019

7:30 AM Registration | Breakfast

Keynote

8:30 AM Next-Generation Batteries

George Crabtree, Argonne National Laboratory

Session VII: Batteries Recycling (Chair: Liu Gao)

9:30 AM The ReCell Center: DOE's Advanced Battery Recycling Program

Bryant Polzin, Argonne National Laboratory

10:00 AM Break (30 mins)

10:30 AM Manufacturing with Recycled Materials

Joon Kim, Spear Power

11:00 AM Quality Assessment for Used Batteries

Shriram Santhanagopalan, National Renewable Energy Laboratory

11:30 AM Electro-Assisted Recycling of Lithium Ion Batteries

Luis Diaz Aldana, Idaho National Laboratory

12:00 PM Lunch (1 hour)

NREL Tour Preparation

1:15 PM Everyone on board the bus

1:40 PM Pick up badges

2:00-4:00 PM NREL tours

Tour 1 Energy Integration Systems Integration Facility (ESIF)

Tour 2 Process Development and Integration Laboratory (PDIL)

After the tour, transportation is provided back to the hotel.

Keynote Speakers



Martin Keller, Ph.D.

Director, National Renewable Energy Laboratory

Martin Keller became the National Renewable Energy Laboratory's (NREL) director on November 30, 2015. NREL is operated for the U.S. Department of Energy (DOE) by Alliance for

Sustainable Energy, LLC (Alliance). Martin also serves as the President of Alliance.

Martin joined Oak Ridge National Laboratory (ORNL) in July 2006 and was appointed to the role of Associate Laboratory Director in July 2009. In November 2010, he was asked to lead the newly formed Energy and Environmental Sciences directorate. In this role he was responsible for the energy, biological, and environmental research programs supported by DOE, the Environmental Protection Agency, and the National Institutes of Health. Martin served as the Founding Director of the DOE BioEnergy Science Center and served as the Director of the Biosciences Division.

Martin held a series of research management positions within Diversa Corporation, a publicly traded biotechnology company. Martin joined Diversa Corporation in 1994 as a consultant to build and develop their microbiology expertise before joining Diversa Corporation full time in 1996.

Martin received his Ph.D. in Microbiology from the University of Regensburg, Germany.

Abstract of Martin Keller's Presentation: Transforming Energy through Innovation

These remarks focus on the impacts of global mega trends on America's energy future. Declining costs for renewables and batteries are driving significant changes to our national grid and transportation systems. NREL's advanced scientific research on transforming energy, and the role energy storage plays in this effort, will be discussed.



George W. Crabtree, Ph.D.

Director, Joint Center for Energy Storage Research (JCESR) Argonne National Laboratory University of Illinois at Chicago

George Crabtree is Director of the Joint Center for Energy Storage (JCESR) at Argonne National Laboratory and Professor of Physics, Electrical,

and Mechanical Engineering at University of Illinois-Chicago (UIC). His professional interests include nextgeneration battery technology and its applications in transportation and the electricity grid, as well as integration of energy science, technology, policy and societal decision-making. He has led several workshops for the Department of Energy on energy science and technology, is a member of the National Academy of Sciences, and has testified before the U.S. Congress on the hydrogen economy, on meeting sustainable energy challenges, and on the prospects for next-generation electrical energy storage.



Vincent L. Sprenkle, Ph.D.
Chief Scientist - Energy Storage,
Pacific Northwest National Laboratory

Dr. Vincent Sprenkle joined Pacific Northwest National Laboratory (PNNL) in January 2001 and is the Energy Storage Chief Scientist. He is currently on assignment at the

U.S. Department of Energy – Office of Electricity (OE) supporting R&D activities within the DOE OE Energy Storage Program. From 2014-2018, he served as Technical Group Manager for the Electrochemical Materials and Systems Group at PNNL. Dr. Sprenkle has been active in electrochemical technologies for 25 years and currently holds 23 U.S. patents on fuel cells, batteries, and high temperature electrochemical devices with 22 pending patent applications. He was named PNNL Inventor of the Year in 2014 and Distinguished Inventor of Battelle in 2017. He has been recognized as key contributor on four licensing activities while at PNNL and was awarded the 2017 Green Chemistry Challenge Award from US. EPA with UniEnergy Technologies.

Abstract of Vincent L. Sprenkle's Presentation: Energy Storage for Improved Grid Resilience and Renewables Integration

The ability of the U.S. electric power system to reliably meet customer demand is crucial to our economy and national security. The increasing adoption of variable generation technologies and dynamic changes in customer demand are creating the need for enhanced grid flexibility to ensure the continued reliability, resilience, and security of the electric power system. Batteries and other energy storage technologies that have the capability to both supply and absorb electrical power (bidirectional electrical energy storage) can provide the desired flexibility by buffering electrical supply and demand. Large-scale adoption of energy storage can also support resilience to a growing array of weatherrelated, physical, and cyber threats. This presentation will highlight the potential for grid-scale energy storage to improve grid resiliency and renewables integration along with the technical challenge being addressed by DOE OE's R&D program.

Abstract of George W. Crabtree's Presentation:

Energy storage is at the center of several transformative technologies including electric vehicles, wind and solar electricity, energy management for utilities and customers, replacement of gas peaker plants in the grid, and electric flight for air taxis, package delivery, and short-haul passenger service. These emerging uses require next-generation batteries custom-designed for specific applications. A survey of battery

applications needs in the electricity grid, electric vehicles, and flight and the outlook for batteries that can fulfill them will be given.

This work is supported by the Joint Center for Energy Storage Research (JCESR), an Energy Innovation Hub funded by the Department of Energy, Office of Science, Basic Energy Sciences.

Speaker Biographies

Session 1



Prashant Kumta, Ph.D.

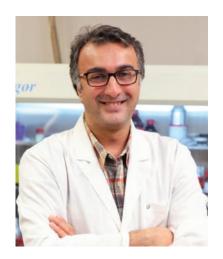
University of Pittsburgh

Professor Kumta obtained his Bachelor of Technology in Metallurgical Engineering from the Indian Institute of Technology, Bombay, India in 1984. He then obtained his M.S. and Ph.D. degrees in Materials Science and Engineering from the University of Arizona in 1987 and 1990, respectively. He joined Carnegie Mellon University as an Assistant Professor in 1990 where he was promoted to Full Professor with tenure in 1999 serving on the faculty of the Department of Materials Science and Engineering and the Department of Biomedical Engineering. He joined University of Pittsburgh in 2007 where he is currently the Edward R. Weidlein Chair Professor in the Swanson School of Engineering and the School of Dental Medicine. He is a Fellow of the American Ceramic Society, as well as the American Institute of Medical and Biological Engineers, and is the former Editor-in-Chief of Materials Science and Engineering, B, Advanced Functional Solid-State Materials, an international journal by Elsevier, and a position he held from 1999-2017.



Jim Zheng, Ph.D. *Florida A&M University and Florida State University*

Dr. Jim P. Zheng is a Professor and Sprint Eminent Scholar Chair at the Department of Electrical and Computer Engineering of Florida A&M University and Florida State University. He is the recipient of the National Academy of Inventors Fellow, National Research Council Fellow, Army Research & Development Achievement Award, NASA Faculty Research Award, and Progress Energy Professional Development Award. He has published over 300 articles in scholarly journals and conference proceedings in the fields of energy storage, fuel cells, nano-sensors, photonics, and thin film growth. He has been awarded 18 patents, and five patents have been licensed by a private company.



Dr. Amin Salehi-Khojin *University of Illinois at Chicago*

Dr. Amin Salehi-Khojin is an Associate Professor in the Department of Mechanical and Industrial Engineering at University of Illinois at Chicago (UIC). He received his Ph.D. in Mechanical Engineering from Clemson University and completed four years of post-doctoral studies in the Department of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign (2008-2012). His research mainly focuses on advanced energy storage and conversion systems. He has co-authored more than 70 journal publications including three papers in *Science*, two in *Nature*, one in *Nature Nanotechnology*, and three papers in *Nature Communications*. He is co-inventor of more than 10 patents/patent applications. His research has been featured in more than 2,000 news releases including Times of London, Guardian, New York Post, Huffington Post, Forbes, Christian Science Monitor, MIT Technology Review, and Chicago Tribune. He was also listed among "Illinois Researchers Who Wowed Us in 2016."



Xiaolin Li, Ph.D.Pacific Northwest National Laboratory

Dr. Xiaolin Li is a senior scientist and technical team lead of battery development and reliability at Pacific Northwest National Laboratory. He received his Ph.D. degree in 2005 from Department of Chemistry, Tsinghua University and conducted his postdoctoral research at Stanford University. He has extensive experience with carbon nanotubes, graphene, and is an expert in designing nanostructured functional materials for various applications. His current research interest is on battery materials and renewable energy. Dr. Li has published many papers in top research journals including Science, Nature Nanotechnology, Nature Communications, Energy Environmental Science and the Journal of the American Chemical Society. His work has resulted in more than 27,000 citations over the years. In 2018, Dr. Xiaolin Li was selected as "the top 1% highly cited researchers." He is the organizer for Nature conference of Materials Electrochemistry: Fundamentals and Applications.

Session 2



Kang Xu, Ph.D.

Adelphi Laboratory Center, Army Research Laboratory

Dr. Kang Xu is a Fellow and Team Leader of the Extreme Electrochemistry Team at the Army Research Laboratory. He received his Ph.D. in Chemistry from Arizona State University (1996), M.S. in Polymer Chemistry from the Institute of Chemical Physics, Academy of Sciences (1988), and B.S. in Chemistry from Southwest University (1985). Xu is Co-founder of the Center of Research on Extreme Batteries, on the Advisory Board of ACS Applied Materials, and is Associate Editor for Energy & Environmental Materials and Electrochemistry. Xu has over 30 years of experience in electrolyte materials, has published over 200 papers, four chapters/books, over 20 patents, 20,000 citations, and an h-index of 72. He is best known in the field for two comprehensive reviews in Chem. Rev. in 2004 and 2014. Xu has received over 20 awards, including the 2017 International Battery Association Technology Award and the 2018 Electrochemical Society Battery Research Award.



Seung-Tae Hong, Ph.D. *Daegu Gyeongbuk Institute of Science and Technology*

Dr. Seung-Tae Hong is a professor of the Department of Energy Science and Engineering at the Daegu Gyeongbuk Institute of Science and Technology, South Korea since 2012. He earned his Ph.D. in solid-state chemistry from Seoul National University in 1994. Prior to working at the university, he had been a Principal Research Scientist at Battery and Corporate R&D Centers, LG Chem Research Park for 12 years, following postdoctoral research positions at Oregon State University and Iowa State University. He specializes in inorganic materials synthesis, ab initio structure determination from powder X-ray diffraction data, and development of electrode materials for rechargeable batteries. His current main research interests include synthetic, structural, and electrochemical studies of electrode materials for multivalent (Mg, Ca, Zn) ion batteries and inorganic solid electrolytes for all-solid Li and Na batteries.

Speaker Biographies

Session 2 (cont'd.)



Kevin Zavadil *Sandia National Laboratory*

Kevin R. Zavadil is a Distinguished Member of Technical Staff in the Material, Physical, and Chemical Sciences Center at Sandia National Laboratories. Kevin manages one of five science thrust research portfolios for the Joint Center for Energy Storage Research, a DOE Energy Innovation Hub. His current research is focused on the material and interfacial science of electrochemical energy storage devices, including lithium and multivalent metal batteries and redox flow batteries.

Session 3



Jason Zhang, Ph.D. *Pacific Northwest National Laboratory*

Dr. Ji-Guang (Jason) Zhang is a Laboratory Fellow of the Pacific Northwest National Laboratory (PNNL). He is the group leader for PNNL's efforts in energy storage for transportation applications and has 28 years of experience in the development of energy storage devices, including Li-ion batteries, Li-metal batteries, Li-air batteries, Li-S batteries, and thin-film solid-state batteries. He was the co-recipient of two R&D 100 awards, holds 23 patents (with another 32 patents pending), and publishes more than 300 papers in refereed journals. He was named the Highly Cited Researcher in 2015, 2017, and 2018 by Clarivate Analytics.



Nitash Balsara, Ph.D. *University of California, Berkeley*

Technology in Kanpur, India in 1982, a master's degree from Clarkson University in Potsdam, New York in 1984, and a Ph.D. from Rensselaer Polytechnic Institute in Troy, New York in 1988. From 1989-1991, he was a postdoctoral researcher, first at the Department of Chemical Engineering and Materials Science at the University of Minnesota, and then at Exxon Research and Engineering Company in Annandale, New Jersey. In 1992, he joined the faculty of Department of Chemical Engineering at Polytechnic University in Brooklyn, New York. In 2000, he accepted the job that he currently holds: a joint appointment as professor of Chemical Engineering at the University of California, Berkeley, and faculty scientist at Lawrence Berkeley National Laboratory. Along with his students and collaborators, he cofounded two battery start-ups, Seeo, Inc. and Blue Current.



Jeff Sakamoto, Ph.D. *University of Michigan*

Jeff Sakamoto has 20 years of experience studying and translating ceramic materials for electrochemical materials into energy technologies for terrestrial and space applications. He was a senior researcher at the Caltech Jet Propulsion Laboratory (2000-2007), a Professor at Michigan State University (2007-2014) and has been a Professor at the University of Michigan since 2014. The Sakamoto group is involved in ceramic material synthesis and processing, electrochemical and mechanical property characterization of super Li-ion conducting, and cathode ceramic oxides. Dr. Sakamoto is a Kavli Frontiers of Science Fellow and was a chair, organizer, speaker, and delegate at National Academy of Sciences Frontiers of Science and National Academy of Engineering Frontiers of Engineering Symposia. Dr. Sakamoto received two Major Space Act Awards from the NASA Inventions and Contributions Board, is the primary contributor on 24 patents, and received the Teacher-Scholar (2013) and Withrow Excellence in Teaching (2009) Awards at Michigan State University.

Andrew Westover, Ph.D. and Nancy Dudney, Ph.D.

Oak Ridge National Laboratory



Andrew Westover is a Staff Scientist in the Chemical Sciences Division at Oak Ridge National Laboratory. He received his Ph.D. in Interdisciplinary Material Science and Engineering from Vanderbilt University in 2016 and his bachelor's degree from Brigham Young University in 2012 with a double major in Physics and Japanese. His field of expertise is all-solid-state Li-ion batteries, the manufacturing and characterization of Li metal, and structural energy storage.



Nancy Dudney is a distinguished researcher and corporate fellow in the Chemical Sciences Division at Oak Ridge National Laboratory. She received her degrees from the College of William and Mary (B.S., Chemistry) and MIT (Ph.D., Ceramic Materials Science and Engineering) and began work at Oak Ridge National Laboratory as a Wigner Research Fellow in the Solid-state Division. Dr. Dudney's research interests include lithium battery materials and architectures, thin film and composite electrolytes, thin film materials for batteries, and mixed ionic-electronic conduction in oxides. She helped pioneer the development of commercial thin-film lithium batteries and continues to utilize thin film processing and materials in her research toward the stabilization of battery interfaces. Dr. Dudney is a fellow of the Electrochemical Society. She has won four R&D 100 awards. Her goal is to promote development of safe and efficient batteries for vehicles and renewable energy.

Speaker Biographies

Session 3 (cont'd.)



Mike Zimmerman, Ph.D. *Tufts University*

Dr. Mike Zimmerman is the Founder and CEO of Ionic Materials, a technology company that has developed the solid polymer electrolyte with a new conduction mechanism for solid-state batteries, and the founder of iQLP, an incubation lab. Mike was also the Founder and CTO of QLP Inc., which developed and commercialized a disruptive polymer for electronics. Mike began his career at AT&T Bell Labs, where he served as a consulting member of technical staff, which is reserved for the top 1% of the technical community. Mike has been a professor at Tufts University for more than 25 years and holds the title of Professor of the Practice. Mike has a Ph.D. in mechanical engineering and applied mechanics from the University of Pennsylvania, a M.S. degree from Massachusetts Institute of Technology in fibers and polymers division, and a B.S. degree from Rensselaer Polytechnic Institute in mechanical engineering.



Marca Doeff, Ph.D.

Lawrence Berkeley National Laboratory

Marca M. Doeff is a senior scientist at Lawrence Berkeley National Laboratory, whose research interests focus on materials for lithium-ion batteries, sodium-ion batteries, and solid-state devices. She obtained a bachelor's degree in Chemistry from Swarthmore College and a Ph.D. in Inorganic Chemistry from Brown University. She is currently the chair of the Battery Division of the Electrochemical Society, a fellow of that society, and a fellow of the Royal Society of Chemistry.



Nick Wu, Ph.D. *West Virginia University*

Dr. Nianqiang (Nick) Wu is currently George B. Berry Chair Professor in the Materials Science Program at West Virginia University (WVU). He is a Fellow of the Electrochemical Society (ECS) and a Fellow of the Royal Society of Chemistry. He was identified in the 2018 Highly Cited Researchers list by Clarivate Analytics (Thomson Reuters). He has received the Benedum Distinguished Scholar Award and the Alice Hamilton Award for Excellence in Occupational Safety & Health. He was the recipient of the WVU Statler College Outstanding Researcher Award. In the past, he served on the ECS Board of Directors and Chair of the ECS Sensor Division. Dr. Wu's research interests lie in photocatalysts and photoelectrochemical cells for environmental and energy sustainability, electrochemical energy storage, and biosensing and photodynamic therapy (precision medicine).



Donald R. Sadoway, Ph.D. *Massachusetts Institute of Technology*

Donald R. Sadoway is the John F. Elliott Professor of Materials Chemistry in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. His B.A.Sc. in Engineering Science and Ph.D. in Chemical Metallurgy are from the University of Toronto. He joined the MIT faculty in 1978. The author of over 170 scientific papers and 30 U.S. patents, his research is on environmentally sound metals extraction technologies and on batteries for grid-scale storage and for electric vehicles. He is the founder of two companies, Ambri and Boston Metal. Online videos of his chemistry lectures hosted by MIT OpenCourseWare extend his impact on engineering education far beyond the lecture hall. Viewed over two million times, his TED talk is as much about inventing inventors as it is about inventing technology. In 2012, he was named by Time magazine as one of the 100 Most Influential People in the World.



Jagjit Nanda, Ph.D. *Oak Ridge National Laboratory*

Jagjit Nanda is a Senior Staff Scientist at Oak Ridge National Laboratory's Chemical Sciences Division, working in the area of high capacity energy storage materials, interfaces, and energy systems. He is a joint faculty professor in the Chemical and Biomolecular Engineering Department at the University of Tennessee. Prior to joining Oak Ridge in 2009, Jagjit was the Technical Expert at the Research and Advanced Engineering Center, Ford Motor Company, leading R&D projects in lithium-ion battery materials and nanomaterials for energy application. Jagjit received his Ph.D. in Solid-state Chemistry & Materials Science from the Indian Institute of Science in 2000 followed by a Postdoctoral Fellowship at Stanford University (2000-02) and an early career research staff (2002-05) at Los Alamos National Laboratory. He has published over 150 journal and technical publications, holds 10 patents in the area of energy storage R&D, and is an active member of several professional scientific societies.



Zheng Li, Ph.D. Virginia Tech

Professor Zheng Li is currently an assistant professor of Mechanical Engineering at Virginia Tech. Prior to joining Virginia Tech, he was a research scientist and postdoctoral researcher at MIT. His research interests center on the design, manufacturing, and electrochemistry of energy storage systems. Professor Li is a serial inventor in the energy storage field. He has led the prototype design of several innovative battery technologies (e.g., aqueous sodium-ion battery, sulfur-based flow battery and lithium-ion battery recycling) at MIT and Virginia Tech. These inventions have resulted in nine patent applications and 23 journal publications. He received his bachelor's degree in Materials Physics at Jilin University, China in 2006 and his master's degree in Materials Science and Engineering at Tsinghua University, China in 2008. He completed his Ph.D. in Materials Science and Engineering in 2011 at the State University of New York at Binghamton.

Speaker Biographies

Session 5



Evan Reed, Ph.D. *Stanford University*

Evan Reed is a faculty member in Materials Science and Engineering at Stanford University. He received a B.S. in applied physics from Caltech (1998) and Ph.D. in physics from MIT (2003). In 2004, he was an Ernest Orlando Lawrence Fellow and staff scientist at Lawrence Livermore National Laboratory before moving to Stanford in 2010. Evan Reed's recent work focuses on theory and modeling of 2D materials, statistical learning for chemical and energy storage applications, structural phase changes, and high-pressure shock wave compression.



Alec Talin, Ph.D.

Sandia National Laboratories

Alec Talin is a Distinguished Member of Technical Staff at Sandia National Laboratories, an Adjunct Associate Professor of Materials Science and Engineering at the University of Maryland and is a Fellow of the American Physical Society. Prior to joining Sandia in 2002, Alec spent 6 years as a research scientist and manager at the Motorola Corporate Labs in Phoenix, Arizona and was a Project Leader at the Center for Nanoscale Science and Technology at the National Institute of Standards and Technology from 2009 to 2012. Currently, Alec leads projects at Sandia in materials and devices for low power computing, energy storage, and national security.



Kevin Roche *IBM Almaden Research Center*

Kevin Roche is an advisory engineer/scientist at IBM Research Almaden, specializing in materials for magnetoelectronics, spintronics, and other related fields. He is an expert in ultra-high-vacuum systems and thin-film deposition, data acquisition, and laboratory automation. A native of the San Francisco Bay Area, Kevin earned his bachelor's degree in Physics at the University of California, Berkeley in 1983. He first joined IBM Research in 1982 as an American Physical Society intern; after completing his degree, he returned to IBM Research. Since 2002, Kevin has been introducing and explicating his work in physics and materials science publicly, making it accessible to audiences with a wide range of technical education; in 2017 he added quantum computing concepts to that role and has been an official IBM Q ambassador since 2018. Kevin is a dedicated science fiction fan. In August 2018, he chaired the 76th World Science Fiction Convention.



Bert de Jong, Ph.D.

Lawrence Berkeley National Laboratory

Bert de Jong is a Senior Scientist at Lawrence Berkeley National Laboratory (LBNL), where he leads the Computational Chemistry, Materials, and Climate Group. Focus areas in his group include quantum computing and high-performance and exascale computing, as well as machine learning for chemical and materials sciences. de Jong is the director of the LBNL Quantum Algorithms Team, the LBNL lead for the Basic Energy Sciences Quantum Information Sciences project and is also part of LBNL's superconducting qubits quantum test bed. de Jong has published over 120 papers and book chapters with over 5,200 citations and an h-Index of 32. He published one edited book and has given over 80 invited presentations and lectures at international conferences and universities. de Jong is the Founding Editor-in-Chief for the IOP journal Electronic Structure and a Specialist Editor for Computer Physics Communications.

Session 6



Jordi Cabana, Ph.D.
University of Illinois at Chicago

Jordi Cabana is an Associate Professor at the Department of Chemistry of the University of Illinois at Chicago (UIC) and a member of the Joint Center for Energy Storage Research. Prior to his appointment at UIC, he was a Research Scientist at Lawrence Berkeley National Laboratory from 2008 to 2013. Professor Cabana completed his Ph.D. in Materials Science at the Institut de Ciència de Materials de Barcelona, Spain in 2004, followed by a postdoctoral appointment in the Department of Chemistry at Stony Brook University. He is generally interested in the physical and inorganic chemistry of materials for electrochemical applications, with emphasis on redox and transport properties. He was designated "Up-and-Coming" by Chemistry of Materials in 2017. He is currently a Scialog Fellow in Advanced Energy Storage, and he received a Scialog Award in 2018.



Maxwell Giammona, Ph.D.

IBM Almaden Research Center

chemistries including metal-air batteries.

Maxwell Giammona is a postdoctoral researcher in the energy storage group at IBM's Almaden Research Center in San Jose, California. Max received his Ph.D. in physical chemistry from the University of California, Santa Barbara where he focused on using scanning probe microscopies to understanding the electronic and self-assembly behavior of polymeric systems. His broad research interests are in applying scanning probe and spectroscopic techniques to determining structure-function relationships in materials related to energy storage and clean energy generation. While at IBM Almaden, Max's research has focused on using in-situ atomic force microscopy and other characterization tools to understanding the fundamental physical and chemical behaviors underlying beyond Li-ion battery

Speaker Biographies

Session 6 (cont'd.)



Fulya Dogan, Ph.D. *Argonne National Laboratory*

Fulya Dogan is a staff scientist in the Chemical Sciences and Engineering Division at Argonne National Laboratory. She received her Ph.D. in chemistry from the Stony Brook University with Professor Clare P. Grey in 2011. Her main research interests are applications of solid-state nuclear magnetic resonance to materials of relevance to energy storage and catalysis. Dr. Dogan has expertise in qualitative and quantitative nuclear magnetic resonance methodologies to understand materials' local structure and chemical activity relationships and investigation of surface, interface, and bulk chemistries.



Miaofang Chi, Ph.D.Oak Ridge National Laboratory

Miaofang Chi is a senior staff scientist at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (ORNL). She received her Ph.D. in Materials Science and Engineering from University of California, Davis in 2008. Her primary research interest lies in the advancements and applications of novel electron microscopy techniques in energy and nanotechnology research, especially in the understanding of interfacial charge transfer behavior in energy storage and nanoelectronics systems. She was awarded the Burton Metal by the Microscopy Society of America (2016). She received the ORNL Director's Award for Outstanding Individual Accomplishment in Science and Technology (2015) and the ORNL's Early Career Research Award (2015). Miaofang is the author and co-author of more than 150 peer-reviewed journal articles. She was named to the Clarivate's 2018 list of Highly Cited Researchers.

Session 7



Bryant Polzin *Argonne National Laboratory*

Bryant Polzin has worked at Argonne National Laboratory for the past 9 years in research and development of lithium-ion batteries for transportation applications. He is currently splitting his time as Deputy Director of the ReCell Center (DOE's Advanced Battery Recycling Program) and the Cell Analysis, Modeling, and Prototyping (CAMP) Facility. For the ReCell center, he is providing technical guidance, program support, and outreach. In his CAMP facility work, he has focused on materials evaluation and the scale-up of batteries from coin cell level to xx3450/xx6395 pouch cells and 18650 can cell level. Prior to joining Argonne National Laboratory, Bryant spent 10 years working in industry. He holds a M.S. from Illinois Institute of Technology in Materials Science and Metallurgical Engineering and a B.S. from lowa State University in Ceramic Engineering.



Joon Kim, Ph.D.
Spear Power Systems, Inc.

Dr. Joon Kim founded Spear Power Systems in 2013 after serving as Vice President of Technology at Dow Kokam, LLC since in 2009. He co-founded Kokam America, Inc. in 2005 and served as Chief Technology Officer. Prior to founding Kokam America, Inc., Dr. Kim was Vice President of Li-ion Battery Sales & Marketing at EaglePicher, Inc. He also held various leadership positions for the development of a Li-S rechargeable battery at Sion Power Corporation. Formerly, Dr. Kim was a Staff Research Associate at Lawrence Berkley National Laboratory working on materials for lithium rechargeable batteries. He also was Director of Corporate R&D Analytical Laboratory and a Research Group Leader conducting research on conducting polymers, surface/interface phenomena, and sol gel chemistry at LG Chemical in Korea. Dr. Kim received Ph.D. in chemistry from the University of Illinois at Urbana-Champaign and a B.S. with Cum Laude in chemistry from Seoul National University, Korea.

Shriram Santhanagopalan, Ph.D.

National Renewable Energy Laboratory

Shriram Santhanagopalan leads the Diagnostics and Characterization team in the Vehicle Electrification Group at the National Renewable Energy Laboratory (NREL). Over the last 10 years Shriram has developed models, materials, and test methodology to address performance and safety limitations of batteries. He has worked extensively with several leading battery manufacturers and vehicle original equipment manufacturers around the world. Before joining NREL, Shriram was a Senior Research Scientist at Celgard, LLC, where he was responsible for performing fundamental studies of electrodes, evaluating polymers, developing new characterization tools for large-format batteries, and the design of new Li-2 components for automotive batteries. He actively participates in committees on battery standards. He has authored over 60 peer-reviewed articles and several book chapters, including a book he co-authored with the NREL team. He received his Ph.D. in Chemical Engineering from the University of South Carolina.



Luis Diaz Aldana, Ph.D. *Idaho National Laboratory*

Dr. Luis Diaz Aldana is a scientist engineer-researcher at Idaho National Laboratory (INL). He received his doctorate in chemical engineering from Ohio University and his master's and bachelor's in chemical engineering from Universidad Nacional de Colombia. At INL, his research focuses on the development of low-cost, sustainable, electrochemical processes for metals recovery from used products. As an electrochemical engineer, he applies electrochemistry and chemical engineering principles for the development of processes that transform electrical energy to chemical energy, and vice versa, with low environmental impact. Dr. Diaz is developing a technology that can enable a circular economy for lithium ion batteries, with both lithium and cobalt being returned to battery manufacturers for new Li-ion batteries fabrication. In addition to the electrochemical recycling processes, Dr. Diaz has experience in and has published on the electrochemical conversion of CO2 and the upgrading of organic molecules using electrochemical methods.

Speaker Abstracts



Session 1

Novel Engineering Approaches to High Energy Density Lithium **Metal Batteries**

Prashant N. Kumta, Ph.D. 1,2,3,4

- 1 Department of Chemical and Petroleum Engineering,
- Department of Bioengineering,
- 3 Department of Mechanical Engineering and Materials Science,
- Center for Complex Engineered Multifunctional Materials (CCEMM), Swanson School of Engineering University of Pittsburgh

There is a global demand for high-energy storage systems for portable consumer devices such as cell phones, camcorders, digital videodisk players, and laptops. Coupled with the growing interest in electric vehicles, there has been a major research impetus targeting the generation of high-energy-density rechargeable batteries. Lithium-ion batteries (LIBs) since the commercialization of the first Li-ion battery by Sony in 1991—have emerged as the most promising option due to the high volumetry, gravimetric energy, and power densities. Current LIBs using LiCoO2, LiNiO2, LiMnO4, and LiFePO4 cathodes coupled with a graphite anode exhibit a power density of 100-260 Wh/ kg. There has, therefore, been considerable interest to explore alternative systems for replacing low-capacity carbon anodes with a look back to traditional Li metal and composites. However, Li metal plating on Cu/Li substrates shows undesirable performance due to Li plating instabilities leading to the formation of highsurface-area Li, causing loss of Li due to uneven plating/ deplating, increase in internal resistance, and formation of deleterious Li dendrites. Plating phenomena that is intrinsic to Li metal and copper substrates lead to low coulombic efficiencies, increase in plating/deplating potentials, and consequent hysteresis losses causing rapid fade in specific capacity/energy density, as well as thermal runaway either due to increased internal resistance or internal short circuiting of the cell due to formation and growth of unwanted dendrites. Similarly, lithium-sulfur batteries with a theoretical capacity of 1672 mAh/g utilizing sulfur cathodes have emerged as a promising candidate for high-energy-density battery

system. Furthermore, promising economics, earth abundance, and ease of availability have led to the consideration of sulfur cathodes as an alternative to the hitherto-used transition metal oxide-based cathodes. However, poor electronic conductivity at room temperature and, more importantly, the formation of soluble non-intercalation-based polysulfide species during electrochemical cycling cause significant active material loss by coating onto the anode, resulting in eventual failure of the battery.

This presentation will feature novel strategies of new alloy designs and coating approaches, as well as innovative composite and materials concepts exploiting the interfacial phenomena related to the scientific nuances of electrochemical deposition of lithium. Fundamental mechanisms of nucleation and growth of lithium metal and the underlying interconnectivity of electrochemical deposition of lithium with the substrate structure and interfacial energy will be outlined elucidating an overall pathway towards engineering dendrite-free substrates as nextgeneration high capacity anode materials. Similarly, new approaches to entrapping polysulfide species and enabling high sulfur loadings overcoming the intrinsic limitations of poor kinetics and transport will be described. In doing so, unique paradigms to next-generation high-capacity anode and cathode systems for enabling high-energy-density, lithium metal batteries will be presented and discussed.

Investigate the Formation of Discharge Products to the Limitation of Energy Density in Cathode of Li-S Batteries

Jim. P. Zheng, Ph.D.^{1,3,4}, Chao Shen^{1,3,} Jianxin Xie^{2,5,} Mei Zhang^{2,5,} and Petru Andrei 1,3

- 1 Department of Electrical and Computer Engineering and
- 2 Department of Industrial and Manufacturing Engineering, Florida A&M University and Florida State University
- 3 Aero-Propulsion, Mechatronics and Energy Center,
- Center for Advanced Power Systems, and
- High-Performance Materials Institute, Florida State University

Rechargeable lithium-sulfur (Li-S) batteries with a theoretical specific energy of 2,500 Wh kg-1 are promising candidates to replace Li-ion batteries in many applications.1 Even though Li-S batteries possess a high theoretical specific energy, several major technical challenges must be overcome. Many of these challenges are closely related to the formation of soluble lithium polysulfide (LiPS) intermediates. For instance, the irreversible redistribution of LiPS inside the battery leads to degradation of sulfur cathodes and passivation of Li metal anode. The uncontrolled LiPS relocation further leads to severe active material loss and self-discharge behavior of the batteries.

Ultimately, the most critical question for Li-S batteries is whether their high theoretical energy density can be practically delivered. The practical specific energy of Li-S batteries greatly depends on the electrolyte/sulfur (E/S) ratio of the batteries. To increase the energy density of rechargeable Li-S batteries, the E/S ratio should be decreased as much as possible. However, when the E/S ratio is decreased, multiple issues arise that degrade battery performance, such as discharge capacity, cycle life, and rate capability. Very importantly, our group has recently found that once the electrolyte becomes saturated with liquid phase high-order LiPS, the solid phase LiPS cannot be further reduced and consequently does not contribute to the capacity of the cells at normal discharge rates.2,3 Therefore, the solubility of high-order LiPS can potentially lower the achievable specific energy of Li-S batteries to less than 500 Wh kg-1, which becomes much less attractive for their commercialization.

To address the above-mentioned challenges associated with conventional Li-S batteries, here we use the solidstate lower-order LiPS, i.e., Li2S4, as the cathode active material to construct a new type of Li-Li2S4 battery.4 By replacing the elemental sulfur with solid-state Li2S4 as the active cathode material, we avoid any solubility limitation previously encountered in the upper plateau of discharge. We found that in the lower plateau of discharge, the discharge capacity is not limited by the finite solubility of Li2S4, and much higher discharge capacity with a Li-Li2S4 cell is achieved under a higher sulfur content of 84% and a low E/S ratio of 4.4 ml g-1. Moreover, the cyclability is also enhanced due to the reduced diffusion of high-order LiPS. We believe the reported results of our Li2S4 cathode open a new

direction of cathode development for high-energydensity Li-S batteries.

Insights into New Li-O2 **Electrochemistry Strategies** for Energy Storage

Amin Salehi-Khojin Ph.D. University of Illinois at Chicago

Lithium-ion battery technology has transformed the portable electronics industry and is making inroads into energy storage on the electric grid and electrically powered transportation. Today, research laboratories around the world are pursuing development of beyond-lithium-ion batteries that are even more powerful, cheaper, safer, and longer-lived. One such type of advanced battery is the lithium-air (Li-O2) battery, which is believed to be able to hold up to as much energy as the lithium-ion battery. The Li-O2 battery has been tantalizing to battery researchers in recent years, but several obstacles have plaqued their development. In this talk, I will review some of the recent work on investigations into two types of Li-O2 batteries. The first is on Li-O2 batteries that operate based on formation and decomposition of lithium superoxide, instead of the usual lithium peroxide, as the discharge product. The second is a Li-O2 battery that operates in a realistic air atmosphere, instead of the usual O2 atmosphere, with a long cycle life. The results of experimental and computational studies of discharge and charge chemistries that reveal insight into how these batteries operate will be presented.

Development of High-Performance **Na-Ion Battery Cathodes**

Xiaolin Li, Ph.D., Junhua Song, Biwei Xiao, David Reed, Vincent L Sprenkle Pacific Northwest National Laboratory

Sodium-ion batteries (SIBs), with the intrinsic advantages of resource abundance and geographic uniformity over that of Li-ion batteries (LIBs), are a desired alternative battery technology for grid-scale energy storage and transportation applications. To make SIBs comparable to LIBs in electrochemical performance, it is essential to develop advanced cathode materials of high capacity and long cycle life. Here, we report the synthesis of long-life and high-capacity O3-type layered cathode for practical SIBs. The nickel-rich nickel-manganese-cobalt cathode delivers a specific capacity of ~196 mAh g-1, a specific energy of ~612 Wh kg-1 (based on the cathode), and >83% capacity retention over 100 cycles between 2-4.2V (vs. Na/Na+). The cathode has ~80% capacity retention over 1,000 cycles with a specific capacity of ~151 mAh g-1 between 2-4V. Full-cells with practical loading (>2.5mAh cm-2) and controlled electrolyte amount (~40 µl) also have been demonstrated. The capacity retention is >91% over 200 cycles. In another effort, a high-performance P2-type of cobalt-free cathode also has been developed to deliver ~190 mAh q-1 specific capacity between 1.5-4.4V with 95% retention over 50 cycles.

Session 2

Beyond Li-Ion Chemistries in **Aqueous Electrolytes**

Kang Xu, Ph.D. **Electrochemistry Branch** Sensor and Electron Devices U. S. Army Research Laboratory

When Li-ion chemistries based on transition metal oxide intercalation hosts are gradually approaching their ceilings in many technical parameters, beyond Li-ion chemistries (sodium, potassium, or multivalence ions like zinc and magnesium, etc.) were considered as alternative bypasses to higher energy densities. These efforts have encountered various challenges, with electrolytes being the most frequent obstacles. Replacing non-aqueous solvents with water could bring significant benefits in both safety and environmental friendliness but nonetheless increasing some of the challenges. One such conspicuous challenge has been the electrochemical stability window of water. This talk will summarize our recent efforts in this direction and the various high-voltage, aqueous, beyond-Li-ion chemistries thus enabled.

Intercalation Chemistry of Mg and Ca lons Into Host Materials for Post Li-lon Batteries

Seung-Tae Hong, Ph.D. Dept. of Energy Science and Engineering, DGIST (Daegu Gyeongbuk Institute of Science and Technology), Daegu, Korea

Li ion batteries (LIBs) are one of the most successful energy storage devices for portable electronics application, electrical vehicles, and utility grids. However, there are still strong needs for higher energy density and lower price materials than what the LIB systems can provide. Environmental friendliness, reliability, safety, and plentiful sources could be typical advantages of magnesium (Mg) and calcium (Ca) over the lithium. Rechargeable batteries utilizing intercalation of divalent ions such as Mg2+ and Ca2+ could be one of the strategies to overcome the capacity limit of LIBs, and/or to produce lower price batteries. Mg rechargeable batteries have received attention since the reversible Mg intercalation into the Chevrel phase, Mo6S8, was demonstrated in 2000. Very recently, Ca-based rechargeable batteries have also received attention. However, only a limited number of materials have been reported for the successful host materials that can intercalate such divalent ions reversibly. The electrochemical intercalation chemistry is one of the emerging research fields for future batteries. In this talk, recent progress in our exploration for new intercalation chemistry of such divalent ions into various host materials will be presented, utilizing aqueous electrolytes as well as non-aqueous electrolytes.

Multivalent Anode Interphases: Opportunities to Direct Interfacial **Cation Transport**

K.R. Zavadil Sandia National Laboratories

Regulating cation transmission at electrode interfaces is an essential function required for realizing storage based on multivalent working ions, including magnesium and calcium. Cation transmission regulating interphases are believed to exist at the anode surface for a host of electrolytes, impacting the Coulombic efficiency, deposition/dissolution rates, and achievable capacity (stability) of metal deposits. These interphases are derived from supporting electrolyte anion, solvent or impurity decomposition, or more complex synergistic reactions. Recently developed, weakly coordinating anions, of defined reductive stability in highly purified form, provide a unique opportunity to systematically explore the origin, identity, and properties of formed interphases. In this presentation, we describe the correlation between bulk electrolyte speciation, interfacial speciation, and subsequent reactivity. We demonstrate how the interphase can be manipulated through exploiting a deeper knowledge of the electrolyte. Our results highlight critical phases and distributions responsible for cation transport and provide new insight into directing interphase formation to facilitate cationtransport-enhancing electrode performance.

This work was supported as part of the Joint Center for Energy Storage Research, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

Session 3

Non-Flammable Electrolytes for Lithium Metal Batteries

Ji-Guang Zhang, Ph.D. Pacific Northwest National Laboratory

Rechargeable lithium (Li) metal batteries (LMBs) have been regarded as the "holy grail" of energy storage systems because of the unique advantages of Li metal anode (LMA). Unfortunately, rechargeable batteries based on LMAs have not yet been commercialized due to several barriers. In the late 1980s, commercialization of LMBs was hindered because of safety concerns. In this work, we will demonstrate several fire-retardant localized high concentration electrolytes that enable stable, dendrite-free cycling of LMAs with high coulombic efficiency of up to 99.2%. Moreover, this electrolyte exhibits excellent anodic stability even up to 5.0 V and greatly enhances the cycling performance of LMBs. A Li|| LiNi0.6Mn0.2Co0.2O2 battery using this electrolyte can retain > 97% capacity after 600 cycles at 1C rate (ca. 1.6 mA cm-2), corresponding to a negligible capacity decay of < 0.005% per cycle. These nonflammable electrolytes are not only stable with LMAs but also can enable safe operation of Li ion batteries based on the silicon anode. Therefore, they will have broad application for rechargeable Li batteries.

Predicting the Performance of Lithium Metal Electrodes Stabilized by Polymer Electrolytes

Nitash P. Balsara, Ph.D., Danielle M. Pesko University of California, Berkeley

It is now commonplace to report the data obtained during cycling of symmetric cells with solid polymer electrolytes. The parameter that is usually the focus is the number of cycles prior to cell failure. Quantitative

prediction of cell failure is a daunting task. As a step toward that aim, we seek to predict the potential needed to cycle such cells at a function of the applied current density. We show that such predictions cannot be made on the basis of knowledge of conductivity alone. The importance of complete characterization of polymer electrolytes will be discussed. This includes determination of the thermodynamic factor, salt diffusion coefficient, and transference number. The connection between these parameters and dendrite growth is being explored. If new results are obtained, I will present them at the meeting.

Electrochemical, Quantum Mechanical, and Physical Behavior of the Li Metal-Solid Electrolyte Interface

Professor Jeff Sakamoto, Ph.D. University of Michigan

There is tremendous interest in making the next super battery, but state-of-the-art Li-ion technology works well and has inertia in several commercial markets. Supplanting Li-ion will be difficult. Recent material breakthroughs in Li metal solid-state electrolytes could enable a new class of non-combustible solidstate batteries (SSB) delivering twice the energy density (1,200 Wh/L) compared to Li-ion. However, technological and manufacturing challenges remain. The discussion will consist of recent milestones and attempts to bridge knowledge gaps to include:

- Stability and kinetics of the Li metal-solid electrolyte interface
- Understanding and controlling an unusual phenomenon: Li metal penetration in solid electrolytes; how can something soft penetrate something hard?
- Solid-state mechanics of Li metal and composite ceramic electrodes

Despite the challenges, SSB technology is rapidly progressing. Multi-disciplinary research in the fields of materials science, solid-state electrochemistry, and solid-state mechanics will play an important role in determining if SSB will make the lab-to-market transition.

Can Glassy Electrolytes Enable All-Solid-State Li Metal Batteries?

Andrew Westover, Ph.D. and Nancy Dudney, Ph.D., Oak Ridge National Laboratory

A Li metal anode is one of the keys to Li-ion batteries that can reach energy densities beyond 500 Wh/kg and hit fast charging targets. The foremost challenges that must be overcome is the formation of Li filaments that penetrate the separator shorting the battery. This problem is incredibly pervasive limiting performance in liquid, polymer, and ceramic electrolytes. The one key exception to this is in glassy electrolytes, such as lithium phosphorus oxynitride (Lipon) and related compositions. In thin film batteries, these electrolytes completely suppress the formation of Li filaments and can enable pulses of charging up to at least 10 mA/cm2. Understanding what makes these glassy electrolytes work is key to making larger scale batteries that can completely suppress Li filaments and enable fast charging.

Here we will answer three key questions:

- 1. How would Lipon perform if it had interparticle boundaries similar to a ceramic?
- 2. Can a glassy interface suppress Li filament growth in ceramic electrolytes?
- 3. What is the limit of performance for glassy electrolytes?

Acknowledgements: This work was supported by the ARPA-E IONICS program, U.S. Department of Energy, award DE-AR0000775.

Enabling Solid-State Batteries with Breakthrough Polymer Technology

Mike Zimmerman, Ph.D. **Tufts University**

We will present a new polymer electrolyte material that enables safe solid-state batteries that are operational at room temperature and compatible with a handful of widely desired, next-generation battery chemistries, including safe lithium ion, lithium metal, rechargeable alkaline and more.

Benefits of this solution include:

- Inherent safety: eliminates safety issues with liquid electrolytes
- Higher performance: enables higher energy anodes and cathodes
- Lower cost: reduces battery cost through less expensive chemistries and novel manufacturing
- New chemistries: such as rechargeable alkaline

By enabling the creation of batteries that are safer, cheaper, and higher performing than the current state-of-the-art, lonic's polymer electrolyte shatters the traditional battery design paradigm, under which safety, cost, and performance must generally be traded off against one another. The company is bringing this technology to market with core manufacturing partners in the battery industry. The presentation will provide inside access to data and use cases for polymer electrolyte battery solutions.

Towards Solid-State Batteries with LLZO

Marca M. Doeff. Ph.D. *Lawrence Berkeley National Laboratory*

Variants of Li7La3Zr2O12 (LLZO) are widely recognized to be among the most promising solid electrolytes for battery applications, based on their high-ionic

conductivities (> 1 x 10-4 S/cm), wide voltage stability windows approaching 6 V, and good chemical stability. Earlier reported problems associated with high interfacial impedances between lithium metal and LLZO have largely been solved, in part by recognizing the importance of removing highly resistive Li2CO3 layers on LLZO surfaces. The next challenge involves the design of composite cathodes, which are necessary to overcome transport limitations of the active material and to realize high practical energy densities. We are currently exploring freeze tape-casting (FTC) as a scalable, eco-friendly method for generating LLZO scaffolds with highly aligned, low-tortuosity pores, which can subsequently be infiltrated with active materials and other components to form the composite. Freestanding scaffolds about 100 µm thick can be made using this technique, but it is more convenient to produce supported structures in the form of dense/porous bilayers or even porous/dense/ porous trilayers. In both structures, a thin dense layer (ideally no more than about 20 µm thick) serves as the ionically conductive separator. In the bilayer, a thin lithium foil is added as the anode while in the trilayer, either lithium metal or a suitable anode material such as Li4Ti5O12, is infiltrated into the second porous layer to form solid-state cells. For this presentation, we will present our progress in this area, and discuss the challenges that remain.

Ceramic-Polymer Composite Electrolytes for Lithium-Metal Batteries

Niangiang Wu, Ph.D. West Virginia University

The presentation deals with the solid-state ceramicpolymer composite electrolytes in which the lithiumion conducting ceramic nanofiber networks is incorporated into a lithium-ion conducting polymer matrix. The lithium transport pathways in the composite electrolyte has been investigated. The results show that the interface between the ceramic and the polymer plays a significant role in lithium transport. The

optimized composite electrolyte is interfaced with the lithium metal anode, showing the suppression of the lithium dendrite formation.

Session 4

Liquid Metal/Molten Salt Batteries for Stationary Storage

Donald R. Sadoway, Ph.D. John F. Elliott Professor of Materials Chemistry, Massachusetts Institute of **Technology**

Massive-scale electricity storage would offer huge benefits to today's grid, reducing price volatility, improving stability against loss of power, increasing utilization of generation assets by enabling us to design towards average demand instead of peak demand and deferring the costs of upgrading existing transmission lines. When it comes to tomorrow's grid, storage is key to widespread integration of renewables, i.e., solar and wind, which due to their inherent intermittency, are by themselves incapable of being fully integrated into baseload generation. The liquid metal battery is presented as a first solution that comprises two liquid metal electrodes and a molten salt electrolyte. The device offers colossal current capability and long service lifetime at very low cost, i.e., the price point of the electricity market. The round-trip efficiency of these batteries is greater than 80% under daily 4 h discharge (C/4). Fade rates of 0.00009%/cycle have been measured, which implies retention of >99% of initial capacity after 10 years of daily cycling at full depth of discharge. Beyond the liquid metal battery, the liquid displacement battery is offered as a second solution. Unlike the antecedent sodium-nickel-chloride battery chemistry, which is held back by reliance on a fragile, brittle membrane of β'' -Al2O3, the liquid displacement battery achieved uses a porous, electronically conductive membrane, such as a metal mesh, that achieves selectivity by preferred faradaic reaction.

Enabling Redox Flow Battery Chemistries for Long Duration **Energy Storage: Challenges and Opportunities**

Jagjit Nanda, Ph.D. Oak Ridge National Laboratory

Electrochemical energy storage is the key enabler for increased penetration of renewable energy, such as solar and wind, into the electric grid. With growing demand for low-cost and durable large-scale energy storage for multiple markets, such as data storage centers, remote islands, military locations, and the electric grid, emphasis has been on finding relevant chemistries and systems for long duration energy storage. In this context, Redox flow batteries (RFBs) are promising energy storage devices for grid-level applications due to their extraordinarily long cycle life and the ability to independently scale their energy and power densities. Several RFB chemistries utilizing both aqueous and non-aqueous electrolytes have been developed recently. However, in general, agueous RFBs have low operating potentials ca. 1.5 V, resulting in poor energy densities (25 – 30 Wh/kg for an all vanadium RFB), whereas systems containing organic electrolytes with wider electrochemical windows have moderately higher energy densities. The talk will highlight a new approach that uses mediated electrochemical reactions involving anion radical species to chemically mediate high capacity electrodes in a redox flow configuration. As a proof of principle, we show reversible electrochemical activity using two organic anion radicals that mediate a high capacity anode, red phosphorus yielding about 1500 mAh/g within the state-of-charge window. The second part of the talk will focus on current challenges and progress in developing mechanically robust high ion-conducting membrane separators for non-aqueous RFBs.

Acknowledgement

This work conducted at Oak Ridge National Laboratory is supported by Energy Storage Program, Office of Electricity, US Department of Energy and Laboratory Directed Research and Development Program at Oak Ridge National Laboratory.

Sodium-Sulfur Flow Batteries for Low-Cost Stationary Energy Storage

Prof. Zheng Li, Ph.D. Virginia Tech

The existing baseload nuclear and fossil fuel power generation plants are most efficient and long-lived when operated at constant output while renewable energy generation technologies, such as wind and solar, suffer from intermittency. There is an unmet need for low-cost efficient energy storage at gigawatthour scale capacity to improve the efficiency of the conventional power plants and facilitate the growth and integration of renewable energy. Although pumped hydroelectric storage and underground compressed air energy storage have the lowest installation costs today (~US\$100/kWh), each faces geographical and environmental constraints that may limit further deployment. Electrochemical battery systems are particularly promising energy storage technologies that would transform global energy supply and meet long-term performance and cost requirements for large-scale grid energy storage. Among available battery technologies, flow batteries possess an attractive architecture for grid-scale storage due to their ability to decouple stored energy from power, inherent scalability, and potentially low cost. In addition, the scale-up of battery production and the wider adoption of battery technologies require low-cost and high-energy-density battery systems using abundant materials without resource constraints. Herein, we propose several new stationary energy storage technologies that take advantage of highly abundant and versatile sodium (Na) and sulfur (S) chemistries in flow battery architecture. First, we will demonstrate and analyze a new Na-S flow battery utilizing molten S metal and flowable sulfur-based suspension as electrodes. Unlike the conventional flow battery and the high-temperature Na-S battery, the proposed flow battery system decouples the energy and power thermal management by operating at different temperatures for the storage tank (near room temperature) and the power stack (100-150 °C). Second, we will explore new Na- and S-based cathode system by synergistically incorporating alternative abundant elements. The new cathode system can be integrated in flow battery architecture and address critical challenges associated with sulfur shuttle effect.

Session 5

Identification of 11 New Solid Lithium-Ion Conductors with Promise for Batteries Using Data **Science Approaches**

Austin Sendek, Ekin Dogus Cubuk, Qian Yang, Yi Cui, Evan Reed, Ph.D. **Stanford University**

We discover many new crystalline solid materials with fast single crystal Li ion conductivity at room temperature, discovered through density functional theory simulations guided by machine learningbased methods. The discovery of new solid Li superionic conductors is of critical importance to the development of safe all-solid-state Li-ion batteries. With a predictive universal structure-property relationship for fast ion conduction not well understood, the search for new solid Li-ion conductors has relied largely on trial-and-error computational and experimental searches over the last several decades. In this work, we perform a guided search of materials space with a machine learning (ML)-based prediction model for material selection and density functional theory molecular dynamics simulations for calculating ionic conductivity. These materials are screened from over 12,000 experimentally synthesized and characterized candidates with very diverse structures and compositions. When compared to a random search of materials space, we find that the ML-guided search is 2.7 times more likely to identify fast Li-ion conductors, with at least a 44 times improvement in the log-average of room temperature Li-ion conductivity. The F1 score

of the ML-based model is 0.50, 3.5 times better than the F1 score expected from completely random guesswork. In a head-to-head competition against six Ph.D. students working in the field, we find that the ML-based model doubles the F1 score of human experts in its ability to identify fast Li-ion conductors from atomistic structure with a 1,000-fold increase in speed, clearly demonstrating the utility of this model for the research community. In addition to having high-predicted Li-ion conductivity, all materials reported here lack transition metals to enhance stability against reduction by the Li metal anode and are predicted to exhibit low electronic conduction, high stability against oxidation, and high thermodynamic stability, making them promising candidates for solid-state electrolyte applications on these several essential metrics.

Neuromorphic Computing with the Redox Transistor

A. Alec Talin, Ph.D. Sandia National Laboratory

Inspired by the efficiency of the brain, CMOS-based neural architectures and memristors are being developed for pattern recognition and machine learning. However, the volatility, design complexity and high supply voltages for CMOS architectures, and the stochastic and energy-costly switching of memristors complicate the path to achieve the interconnectivity, information density, and energy efficiency of the brain using either approach. In my talk, I will review the latest advances in neuromorphic computing architectures based on deep neural networks implemented using CMOS and memristors and describe the challenges in achieving both high accuracy and energy efficiency using these devices. I will then discuss an alternative approach based on the redox transistor: a device with a resistance-switching mechanism fundamentally different from existing memristors involving the reversible, electrochemical reduction/oxidation of a material to tune its electronic conductivity. I will first describe an inorganic redox transistor based upon the intercalation of Li-ion dopants into a channel of a Li

intercalation material, such as LixCoO2, a common Li intercalation material, or LixMoO3, a two-dimensional layered oxide. These Li-ion synaptic transistors for analog computing switch at low voltage (mVs) and energy display hundreds of distinct, non-volatile conductance states and achieve high classification accuracy when implemented in neural network simulations. I will also discuss a redox transistor based on the polymer system PEDOT:PSS, and which we also call the electrochemical neuromorphic organic device (ENODe). Plastic ENODes are fabricated on flexible substrates enabling the integration of neuromorphic functionality in stretchable electronic systems. Mechanical flexibility makes ENODes compatible with three-dimensional architectures, opening a path towards extreme interconnectivity comparable to the human brain. Finally, I will demonstrate how these elements can be integrated into functional neuromorphic computing arrays.

Fundamentals of Quantum Computing: An Introduction for **Engineers and Scientists**

Kevin Roche IBM Almaden

Quantum Computing has moved from the regime of basic physics research into working technology, albeit one still very early in its development, that holds the exciting promise of solving problems inaccessible to solution by classical (von Neumann architecture) devices. This talk will introduce the fundamental concepts behind quantum computing and some examples of work being done already with today's NISQ (Noisy Intermediate Scale Quantum) processors, with an eye towards development of future fault-tolerant universal quantum computers. This presentation will be non-rigorous (no calculations) and aims to be understandable to an audience of varied technical backgrounds.

Quantum Computing as a Platform for Scientific Discovery in Chemical Sciences

Bert de Jong, Ph.D. Lawrence Berkeley National Laboratory

In recent years significant advances have been made to deliver quantum computing as a platform enabling scientific discovery. One of the early fields to adopt this technology is chemical sciences. While progress has been made in hardware, software, and algorithms, much work is still to be done to make scientific quantum computing a reality. I will discuss the current state-of-the-art in quantum computing and show some examples relevant to the conference, and I will outline some of the open challenges. I will discuss some of the advances made by the Quantum Algorithms Team led out of Lawrence Berkeley National Laboratory, an integrated team of quantum algorithm developers, mathematicians, and computer scientists with a mission to deliver algorithmic, computational, and mathematical advances to enable scientific discovery in chemical sciences on quantum computers.

Session 6

Measuring and Defining Electrochemical Reactions of Transition Metal Oxides In Mg Electrolytes

Jordi Cabana, Ph.D. University of Illinois at Chicago

Electrochemical energy storage was an important enabler of the wireless revolution, and it is touted as a key component of a society that shifts away from its dependence on fossil fuels. Li-ion batteries are the primary technology when high energy devices are required. However, despite their improved functionality over older systems (e.g., lead-acid car batteries), they do not quite yet meet the emerging energy demands in transportation and grid markets. This roadblock sparked interest in the development of batteries that utilize magnesium (Mg) 2+ as ionic carrier. Theoretical predictions indicate that couples exist between a Mg metal negative electrode and oxide positive electrodes that could surpass the current practical limits of current devices. Among the candidate oxides, layered V2O5 and the general family of spinel-type transition metal (M) 2O4 are considered as leading candidates for the reversible intercalation of ions such as Mg2+1,2, the critical reaction in the positive electrode. However, experimental validation, while incipient³, has not been fully achieved. In this talk, we will present the most up-to-date insight into the ability of oxides to diffuse and reversibly intercalate Mg2+. In this task, the ability to synthesize particles at small dimensions is vital, as is the characterization of chemical and physical phenomena using a combination of tools providing information at different scales. We will rely on data from X-ray diffraction, spectroscopy and scattering, electron microscopy, and nuclear magnetic resonance to probe the reactions that occur when oxides are used as working electrodes in cells with electrolytes containing Mg2+. The rationale for the choice of techniques and the key pieces they provided to complete the picture will be discussed. Our ultimate aim will be to establish relationships between crystal-chemistry, charge carrier, and outcomes of the electrochemical reaction.

- 1 M. Liu et al., Energy Environ. Sci. 2015, 8, 964.
- 2 G. Gershinky et al., Langmuir 2013, 29, 10964.
- 3 C. Kim et al., Adv. Mater. 2015, 27, 3377.

In-Situ Electrochemical Atomic Force Microscopy: A Powerful Tool for **Understanding Metal-Air Batteries**

Maxwell Giammona, Ph.D. IBM Almaden

Non-aqueous metal-air (M-O2) batteries are one of the most promising emerging technologies to replace Li-ion batteries due to their very high theoretical energy densities. In order to develop these chemistries into viable products, a complete and fundamental understanding of their operation is required, and one of the best ways to develop that understanding is through the application of in-situ characterization techniques. In the case of M-O2 batteries, in situ observation of electrochemical reactions can be challenging due to a constantly changing electrode surface under highly sensitive conditions. In the first part of my talk, I will report on the development at IBM Almaden of an insitu atomic force microscopy (AFM)-based analytical technique for the characterization of M-O2 battery electrodes, including the design, fabrication, and successful operation of a sealed AFM cell operating in a controlled atmosphere. In the second part of the talk, I will show the results of two studies performed using this new tool. First, we show that depending on the specific water content and lithium salt used in the liquid electrolyte, the discharge product morphology of lithium-air batteries can differ radically. Second, we show that water content and solvent purity play a key role in the chemical stability of the discharge products in sodium-air batteries, with these factors thus being key to limiting self-discharge.

Solid-State NMR Applications on **Rechargeable Battery Chemistries**

Fulya Dogan, Ph.D. **Argonne National Laboratory**

Researchers worldwide are searching for new electrochemical energy storage materials that meet high energy density, life, cost, and safety requirements of batteries for applications like transportation. The strategies for developing new chemistries with higher energy density, stability and safety concerns involve mitigating the problems of existing materials and understanding the structural changes and their relation to material activity, which can lead to characterizationassisted materials synthesis. Therefore, observation of local environment changes and ion dynamics within the bulk and interface and the interaction of the active materials with electrolytes/binders is crucial. Solidstate nuclear magnetic resonance (NMR) is one of

the few structural probes currently available that can quantitatively characterize local environment changes, "see" lattice and non-lattice species, separate dopants from coatings and real-time surface formations, and understand cation dynamics correlating structural changes with electrochemical activity. This overview talk will focus on applications of multinuclear solidstate NMR spectroscopy to study the evolution of surface, interface and bulk on surface-treated cathodes through 27Aluminum NMR, ion dynamics in bulk magnesium (Mg) battery materials through 25Mg NMR, and chemical reactions between the silicon anodes and common electrolyte solvents and binders through 7lithium and 29silicon NMR.

Understanding Conductivity and Stability of Interfaces in All Solid-State Batteries via STEM

Miaofang Chi, Ph.D. Oak Ridge National Laboratory

All solid-state batteries are considered as one of the primary battery configurations that offers costeffective and efficient energy storage. Recently, several solid electrolyte materials have demonstrated ionic conductivities that are equivalent to that of organic liquid electrolytes. Low ion conductivities that were previously believed to be the major issue impeding the use of solid electrolytes are no longer the bottleneck. Rather, their interfaces are frequently found to limit the performance of all solid-state batteries. These interfaces include both internal interfaces, such as grain boundaries and the interfaces between two electrolytes if the solid electrolyte is a composite or a multilayered material. The associated challenges now include electronic conductivity, mechanical integrity, and chemical and electrochemical instabilities that result in limited current densities, inadequate cyclability, and dendrite growth. These phenomena, however, are challenging to characterize and understand since they are often spatially confined and embedded. Owing to its atomic-level spatial resolution for both imaging and spectroscopy, scanning transmission

electron microscopy (STEM) is now a primary technique for addressing the challenges in such studies. In this talk, I will focus on introducing how we use stateof-the-art atomic-resolution STEM and electron energy loss spectroscopy to understand the complex phenomena at interfaces in all solid-state batteries. I will also introduce emerging STEM techniques, such as 4D-STEM-based differential phase contrast imaging and vibrational spectroscopy and discuss how these methods can benefit research of solidstate ionic materials. I will touch on the importance of understanding synthesis mechanisms regarding interfaces by highlighting examples of our recent work aimed at elucidating synthesis and processing mechanisms of solid electrolytes using in situ electron microscopy and neutron scattering.

This work was sponsored by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, the Materials Sciences and Engineering Division and was performed at Oak Ridge National Laboratory's Center for Nanophase Materials Sciences, which is an Office of Science User Facility.

Session 7

The ReCell Center: DOE's Advanced **Battery Recycling Program**

Bryant Polzin Argonne National Laboratory

Lithium-ion batteries in electric and hybrid-electric vehicles are just now starting to reach their end-oflife. There are several options to address these endof-life batteries, landfilling or recycling. Recycling is a desirable option because of the benefits it can bring, including reductions in life-cycle costs, reduced energy usage, lower environmental impacts, and decreased dependence on scarce or imported materials. However, options available now for recycling of lithium-ion batteries are not optimal, so R&D is needed to make economic processes available for use by industry by the time large volumes of batteries from electric vehicles and other uses go out of service.

The Department of Energy's Office of Vehicle Technologies Office has recognized this gap in recycling efforts and has funded a collaboration of three national laboratories and three universities to establish economical recycling processes. The program has four focus areas: Direct Cathode Recycling, Other Materials Recovery, Design for Recycling, and Modeling and Analysis. This talk will cover the location and structure of the ReCell Center, discuss some technological highlights in the different focus areas, and the future direction of the recycling program.

Manufacturing with **Recycling Materials**

Joon Kim, Ph.D. Spear Power Systems, Inc.

The worldwide generation of end-of-life lithium-ion batteries is expected to reach 1.2 million tons per year by 2025. Disposition of batteries relies on tipping fees, and the material recovery is focused on metallic cobalt and nickel. Classic smelting and hydrometallurgical metals refining produces lithium, nickel, and cobalt at similar costs to virgin materials. Manufacturing with these materials is technically and economically similar to manufacturing with virgin materials, and the result is the usual costly lithium-ion cathode anywhere from \$30-\$50/kg. Cathode-healing™ is a low-cost technology for recycling whole electrode materials (<<\$10/kg). For the 1.2 million tons of waste batteries, the opportunity is ~360 thousand tons of cathode with a value ~\$7 billion selling at \$20/kg (compared to ~\$18 billion for classical cathode at \$50/kg). The market could save \$11 billion by employing cathode-healed material in new manufacturing, beyond expensive lithiumion cathodes. To address the opportunity, battery manufacturing must be able to use such recycled materials. This paper discusses manufacturing with positive electrode material produced from cathodehealing methods.

Quality Assessment for Used Batteries

Shriram Santhanagopalan, Ph.D. National Renewable Energy Laboratory

In light of the recent push for direct recycling of lithium-ion cells and lack of consistent metrics to assess quality of batteries for second-use applications, this talk presents some recent progress made at NREL in developing diagnostic tools and analytical tools to characterize properties of lithium-ion batteries at different scales (pack, module, cell, component, and material) to determine the most viable processing routes for used batteries. Examples are presented at each scale to highlight NREL's approach to evaluating used batteries/components. Data from extensive characterization of mechanical and thermal properties of used cell components from experiments spanning multiple years are presented. The presentation also discusses some of the logistical challenges faced by the battery recycling community and the need for consistent guidelines in this global industry.

Electro-Assisted Recycling of Lithium-Ion Batteries

Luis Diaz-Aldana, Ph.D., Josh McNally, John Klaehn, Ningshengjie Gao, Michael Jones, Birendra Adhikari, Tedd Lister Idaho National Laboratory

The fast growth of the electric vehicle (EV) market is generating a continuous anxiety regarding the sources and availability of the minerals required to keep up with an increasing demand of lithium-ion batteries (LIBs). Critical elements (lithium, cobalt, and graphite) are crucial to sustain the manufacturing of EV batteries and consumer electronics. However, the geographical concentration of mining and refining of cobalt and graphite constitute a supply chain risk for the global production of LIBs which, added to technical development, is forcing to a dynamic change

in the battery chemistry. On the other hand, lithium sources are more diverse in nature and geographical distribution. Although the lithium reserves are enough to cover all the scenarios within the next 20 years, the main question is whether the extraction technologies can keep up with the pace of market growth for EV.

LIB recycling is then surging as an alternative that could enable a circular battery economy and stabilize the supply chain of critical materials for LIBs. Industrial processes for the recycling of LIBs are already operating around the world. However, those processes are almost exclusively focused on the recovery of cobalt, nickel and manganese from battery cathodes as the most valuable metals in the LiBs. Hydrometallurgical processes are proposed for a comprehensive recovery that includes lithium. Nevertheless, the high operative costs associated with intensive chemical consumption do not allow a cost-effective recovery of Li at industrial level.

To target this issue, an electro-assisted reducing technology, based on the use of electrons as green reagent, has been proposed for the extraction and recovery of critical materials from LIBs. Through this process, high extraction efficiencies (>98%) can be achieved at solid to liquid ratios up to 120 g/L and in a peroxide free environment. The process is suitable to different battery chemistries and allows the recovery of graphite as a by-product. Description of the process and a flowsheet that allows a comprehensive recovery of different value streams will be discussed.

