

# SYMPOSIUM ES6

Mechanics of Energy Storage and Conversion—Batteries,  
Thermoelectrics and Fuel Cells  
April 18 - April 20, 2017

## Symposium Organizers

Palani Balaya, National University of Singapore  
Jianlin Li, Oak Ridge National Laboratory  
Partha Mukherjee, Texas A&M University  
Kejie Zhao, Purdue University

## Proceedings Statement

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\* Invited Paper

SESSION ES6.1: Ionic Conductors  
Session Chairs: Jianlin Li and Kejie Zhao  
Tuesday Morning, April 18, 2017  
PCC North, 200 Level, Room 228 A

### 10:30 AM \*ES6.1.01

**Mechanical Properties and Their Relationship to Electrochemical Properties through Defect Equilibria of Ion Conducting Materials** Eric D. Wachsman; University of Maryland, United States.

### 11:00 AM ES6.1.02

**Anion-Frenkel Defect Pair as Dominant Source for O Ion Conductions in Pyrochlore Type SOFC** Mingzi Sun; Hong Kong Polytechnic University, Hong Kong.

### 11:15 AM ES6.1.03

**Ab Initio Modeling of Strain Effects on Lithiation of Vanadium Pentoxide** Casey N. Brock; Vanderbilt University, United States.

### 11:30 AM ES6.1.04

**Influence of Defect Induced Lattice Distortion on Vibrational Dynamics and Ionic Transport in Doped Perovskites** Janakiraman Balachandran; Oak Ridge National Laboratory, United States.

### 11:45 AM ES6.1.05

**Mechanical Properties of Oxide Based Li-Ion Conducting Solid Electrolytes** Jeff Wolfenstine; Army Research Laboratory, United States.

SESSION ES6.2: Solid-State Batteries I  
Session Chairs: Jianlin Li and Partha Mukherjee  
Tuesday Afternoon, April 18, 2017  
PCC North, 200 Level, Room 228 A

### 1:30 PM \*ES6.2.01

**Atomic Scale Simulations of Solid Electrolytes—Mechanical Properties and Beyond** Donald Siegel; University of Michigan, United States.

### 2:00 PM ES6.2.02

**Electrochemical Force Microscopy—Probing Local Diffuse Charge Dynamics and Electrochemical Processes at the Solid Liquid Interface** Liam Collins; Oak Ridge National Laboratory, United States.

### 2:15 PM ES6.2.03

**Dynamic Nano-Indentation Studies to Probe Solid Electrolyte/Lithium Interfaces** Erik G. Herbert; Michigan Technological University, United States.

### 2:30 PM \*ES6.2.04

**Mechano-Electrochemical Aspects in Solid-State Batteries** Jeff Sakamoto<sup>1,2,3</sup>; <sup>1</sup>University of Michigan, United States; <sup>2</sup>University of Michigan, United States; <sup>3</sup>University of Michigan, United States.

### 3:00 PM BREAK

SESSION ES6.3: Cathode  
Session Chairs: Craig Arnold and Partha Mukherjee  
Tuesday Afternoon, April 18, 2017  
PCC North, 200 Level, Room 228 A

### 3:30 PM ES6.3.01

**In Situ Mapping and Dynamic Investigation of State-of-Charge Mechanics in Lithium Ion Batteries** Yongjie Hu; University of California, Los Angeles (UCLA), United States.

### 3:45 PM \*ES6.3.02

**A Multiscale Approach to Cathode Design Based on Mapping Intercalation Gradients within Individual Particles and across Particle Aggregates** Sarbajit Banerjee; Texas A&M University, United States.

### 4:15 PM ES6.3.03

**Mechanism of Secondary Particle Disintegration in  $\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{Co}_{0.2}\text{O}_2$  Electrode Caused by Electrochemical Cycle** Rong Xu; Purdue University, United States.

### 4:30 PM \*ES6.3.04

**Effects of Mechanical Stress on Electrochemical Performance in Lithium-Ion Batteries** Craig B. Arnold; Princeton University, United States.

SESSION ES6.4: Poster Session I  
Tuesday Afternoon, April 18, 2017  
8:00 PM - 10:00 PM  
Sheraton, Third Level, Phoenix Ballroom

### ES6.4.01

**Thermoelectric Properties of High-Performance and Flexible  $\text{Cu}_2\text{Se}$  Thin Films Fabricated by Wet-Deposition Methods** Courtney Hollar; Boise State University, United States.

### ES6.4.02

**New MOF-Modified Nitrogen-Doped Graphene ORR Catalyst Synthesized By Nanoscale High Energy Wet Ball Milling** Shiqiang Zhuang; New Jersey Institute of Technology, United States.

### ES6.4.03

**Tuning Thermocell Power Performance Using Forced Convection** Ali Hussain Kazim; Georgia Institute of Technology, United States.

### ES6.4.04

**Novel N and P-Type Half Heusler Compounds for Intermediate Temperature Thermoelectric Energy Conversion** Nagendra S. Chauhan; CSIR-National Physical Laboratory, India.

### ES6.4.05

**Implications of Different Modes of Intrinsic Proton Diffusion in  $\text{BaZrO}_3$  and Y-Doped  $\text{BaZrO}_3$  for High Temperature Proton Conducting Membranes** Foram M. Thakkar; Shell India Markets Pvt. Ltd., India.

### ES6.4.06

**Thermoelectric Energy Conversion in AlN Thin Films Using Electrical Breakdown Process** Dae Yun Kang; Korea University, Korea (the Republic of).

### ES6.4.07

**Desulfurization Materials Based Nano-Adsorbents for Army Logistics Jet Fuel** Dat T. Tran; U.S. Army Research Laboratory, United States.

**ES6.4.08**

**Development of High Temperature Measurement Sensor Using Pyroelectric Ceramic Material** [Jorge L. Silva](#); The University of Texas at El Paso, United States.

**ES6.4.09**

**High-Performance and Flexible Thermoelectric Devices by Screen Printing Colloidal Nanocrystals** [Yanliang Zhang](#); Boise State University, United States.

**ES6.4.10**

**Modelling of the Solid Electrolyte Interface (SEI) Layer to Study Capacity Fade, Aging and Cycle Life of Lithium Ion Batteries Using Kinetic Monte Carlo Approach** [Bjgvan Khanal](#); South Dakota State University, United States.

**ES6.4.11**

**Development of LFCFN System Perovskites as Interconnect and Cathode Materials for SOFCs** [Sai Ram Gajjala](#); Southern Illinois University, Carbondale, United States.

**ES6.4.12**

**Cost and Performance Optimization of Wearable Thermoelectric Devices Based on Human Thermoregulatory Model** [Dimuthu Wijethunge](#); Yonsei University, Korea (the Republic of).

**ES6.4.13**

**Origin of Fast Proton Transport in Stoichiometric Acceptor Doped Perovskites** [Panchapakesan Ganesh](#); Oak Ridge National Laboratory, United States.

**ES6.4.14**

**Electrospun N-Doped Carbon Nanofibers Encapsulating Co Nanoparticles as Efficient ORR Catalyst** [Chaoqun Shang](#); South University of Science and Technology of China, China.

**ES6.4.15**

**Effect of Interfacial Resistance on the Thermal Conductivity of Superlattice Structures of Organic-Inorganic Perovskites** [Rahul Singh](#); Iowa State University, United States.

**ES6.4.16**

**Factors Controlling Surface Oxygen Exchange in Oxides** [Yipeng Cao](#); University of Wisconsin-Madison, United States.

**ES6.4.17**

**Long-Term Cyclic Sealing Performance of a Glass Composite Seal for Solid Oxide Fuel Cells** [Sueng-Ho Baek](#); Myongji University, Korea (the Republic of).

SESSION ES6.5: Anode Materials for Batteries  
Session Chairs: Craig Arnold and Hui-Ming Cheng  
Wednesday Morning, April 19, 2017  
PCC North, 200 Level, Room 228 A

**8:15 AM \*ES6.5.01**

**Mechanical Effects on the Electrode Materials in Li-Ion Batteries during Electrochemical Process** [Joseph Gnanaraj](#); RJ Lee Group, United States.

**8:45 AM \*ES6.5.02**

**Fatigue in High C-Rate Lithium-Ion Anodes with Porous Silicon** [Sibani L. Biswal](#); Rice University, United States.

**9:15 AM ES6.5.03**

**Atomistic Structural Evolution and Li Trapping Due to Delithiation Rates in Si Electrodes** [Kwang Jin Kim](#); Michigan State University, United States.

**9:30 AM ES6.5.04**

**Electrochemical Acoustic Structural Determination of Lithium Ion Batteries** [Daniel Steingart](#); Princeton University, United States.

**9:45 AM ES6.5.05**

**In Situ Measurement of Elastic and Viscoplastic Properties of Lithiated Silicon and Lithium Metal for Li-Ion Batteries** [Luize Scalco de Vasconcelos](#); Purdue University, United States.

**10:00 AM BREAK****SESSION ES6.6: Fuel Cells**

Session Chairs: Sibani Biswal and Jiangyu Li  
Wednesday Morning, April 19, 2017  
PCC North, 200 Level, Room 228 A

**10:30 AM ES6.6.01**

**A Novel Scanning Probe Microscopy Technique for Ultrafast Imaging of Polarization Switching in Ferroelectric and Multiferroic Materials** [Suhass Somnath](#); Oak Ridge National Laboratory, United States.

**10:45 AM ES6.6.02**

**Strain Effects in Surfaces of Doped Ceria for Solid Oxide Fuel Cell Applications** [Aoife K. Lucid](#); Trinity College Dublin, Ireland.

**11:00 AM ES6.6.03**

**Multiscale Modeling of Solid-State Phase Transformations in Metal Hydrides for Hydrogen Storage** [Tae Wook Heo](#); Lawrence Livermore National Laboratory, United States.

**11:15 AM \*ES6.6.04**

**Photo-Induced Ferroelectric Switching in Perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  Films** [Jiangyu Li](#)<sup>1,4</sup>; <sup>1</sup>University of Washington, United States; <sup>4</sup>Chinese Academy of Sciences, China.

**11:45 AM ES6.6.05**

**Grain Boundaries as Hierarchical Phonon Scatters—A Computational Mechanistic Approach** [Stefano F. Leoni](#); Cardiff University, United Kingdom.

SESSION ES6.7: Mechanics in Nano-Structure and Interface  
Session Chairs: Congrui Jin and Jiangyu Li  
Wednesday Afternoon, April 19, 2017  
PCC North, 200 Level, Room 228 A

**1:30 PM ES6.7.01**

**Electrochemical Kinetics and Dimensional Considerations at the Nanoscale** [Prabhakar R. Bandaru](#)<sup>1,2</sup>; <sup>1</sup>University of California, San Diego, United States; <sup>2</sup>University of California, San Diego, United States.

**1:45 PM ES6.7.02**

**Contact Mechanics in Vertical-Contact-Mode Triboelectric Nanogenerators** [Congrui Jin](#); Binghamton University, United States.

**2:00 PM \*ES6.7.03**

**Multiscale Computational Modeling for the Engineering of Rechargeable Batteries** [Alejandro A. Franco](#)<sup>1,2,3</sup>; <sup>1</sup>Université de Picardie Jules Verne - LRCS UMR 7314 CNRS, France; <sup>2</sup>Institut Universitaire de France, France; <sup>3</sup>RS2E, France.

**2:30 PM BREAK**

SESSION ES6.8: Lithium-Sulfur Batteries  
Session Chairs: Congrui Jin and Matt Pharr  
Wednesday Afternoon, April 19, 2017  
PCC North, 200 Level, Room 228 A

**3:30 PM \*ES6.8.01**

**Issues and Potential Solutions in Li/S Batteries** [Perla B. Balbuena](#); Texas A&M University, United States.

**4:00 PM \*ES6.8.02**

**Observation of Dendrite/Separator Interaction in Experimental Li-Ion Battery Cells** [Corey T. Love](#); US Naval Research Laboratory, United States.

**4:30 PM \*ES6.8.03**

**Role of Electrocatalyst in High Energy Density Li-Ion Sulfur Battery** [Leela Mohana Reddy Arava](#); Wayne State University, United States.

SESSION ES6.9: Poster Session II  
Wednesday Afternoon, April 19, 2017  
8:00 PM - 10:00 PM  
Sheraton, Third Level, Phoenix Ballroom

**ES6.9.01**  
**G-Mode KPFM—Bringing Kelvin Probe Force Microscopy into the Information Age** Liam Collins; Oak Ridge National Laboratory, United States.

**ES6.9.02**  
**Probing Separator Defect Geometries and Localized Deposition in Lithium-Ion Batteries** Xinyi M. Liu; Princeton University, United States.

**ES6.9.03**  
**High-Energy X-Ray Scattering Analysis of Structure and Microstrain in Electrochemically Charged  $\delta$ -MnO<sub>2</sub>** Scott T. Mixture; Alfred University, United States.

**ES6.9.04**  
**Electronic Structure and Comparative Properties of LiNi<sub>x</sub>Mn<sub>y</sub>Co<sub>z</sub>O<sub>2</sub> Cathode Materials** Hong Sun; Purdue University, United States.

**ES6.9.05**  
**Structural Characterization of Nanoencapsulated Phase Change Materials Undergoing Thermal Processes** John Shelton; Northern Illinois University, United States.

**ES6.9.06**  
**Thermoelectric Properties of Molybdenum Disulfide (MoS<sub>2</sub>) with Noble Metal Doping** Gilbert K. Kogo; Norfolk State University, United States.

**ES6.9.07**  
**An Mg-Ion Battery Cell Constructed Entirely from Solid-Phase, Flexible Materials** Todd K. Houghton; Arizona State University, United States.

**ES6.9.08**  
**Chemoelastic Response of Two-Dimensional Silicon Lithium-Ion Cathodes** John Berger; Colorado School of Mines, United States.

**ES6.9.09**  
**A Study of Diffusion in Lithium-Ion Electrodes under Fast Charging Using Electrochemical Impedance Spectroscopy** Kazi Ahmed; University of California, Riverside, United States.

**ES6.9.10**  
**Life Expectancy of Lithium Ion Batteries with Silicon Particles in Electrode** Abhishek Sarkar; Iowa State University, United States.

**ES6.9.11**  
**Multiscale Model to Predict Thermal Performance of Lithium Ion Batteries** Abhishek Sarkar; Iowa State University, United States.

**ES6.9.12**  
**Electronic Properties of Organic-Inorganic Halide Perovskite Superlattice Structures** Rahul Singh; Iowa State University, United States.

**ES6.9.13**  
**Three-Dimensional Hierarchical Porous Electrodes for Li-Ion Batteries** Mohammad S. Saleh; Washington State University, United States.

**ES6.9.14**  
**Understanding of Ultralow Thermal Conductivity in Single Crystalline SnSe Thermoelectric Materials** Jiaqing He; Southern University of Science and Technology, China.

**ES6.9.15**  
**Addressing Lithium-Ion Battery Safety and Failure Containment for Modern Grid Energy Storage** Heather M. Barkholtz; Sandia National Labs, United States.

**ES6.9.16**  
**The Study for the Effect of New Cathode on Cell Performance in Molten Carbonate Fuel Cells** Shin Ae Song; KITECH, Korea (the Republic of).

**ES6.9.17**  
**Graphene Coated Nickel Oxide Three-Dimensional Anode for High Capacity Lithium-Ion Batteries** Eunho Cha; University of North Texas, United States.

**ES6.9.18**  
**Toughening of Mg<sub>2</sub>Si Thermoelectric Material by Addition of Nano-SiC Particle** Yasuo Kogo; Tokyo University of Science, Japan.

**ES6.9.19**  
**Optimization for the Thermoelectric Characteristics of Rough Nano-Ridge GaAs/AlAs Superlattice Structures** Chaowei Wu; National Taiwan University, Taiwan.

**ES6.9.20**  
**Thin Flexible Lithium Ion Battery Featuring Graphite Paper Based Current Collectors with Enhanced Conductivity** Xin Lu; Ecole Polytechnique de Montreal, Canada.

**ES6.9.21**  
**Mechanical Properties and Fracture Behavior of Mg<sub>2</sub>Si after Heat Exposure** Takashi Nakamura; Tokyo University of Science, Japan.

**ES6.9.22**  
**A Strategic Approach to Design Binder Free Standing 3D Carbon Nanotubes with High Sulfur Loading for Li-S Batteries** Mumukshu D. Patel; University of North Texas, United States.

**ES6.9.23**  
**Bifunctional 2D TMD Nanocomposites for Oxygen Reduction Reaction and Hydrogen Evolution Reaction** Liangjun Zhou<sup>1,2</sup>; <sup>1</sup>South University of Science and Technology of China, China; <sup>2</sup>Wuhan University, China.

SESSION ES6.10: Solid-State Batteries II  
Session Chairs: Perla Balbuena and Matt Pharr  
Thursday Morning, April 20, 2017  
PCC North, 200 Level, Room 228 A

**8:30 AM \*ES6.10.01**  
**Reliability and Durability of Materials and Components for Solid-State Energy Conversion Systems** Edgar Lara-Curzio; Oak Ridge National Laboratory, United States.

**9:00 AM ES6.10.02**  
**Controlling the Microstructure of Polycrystalline Li<sub>7</sub>La<sub>2</sub>Zr<sub>2</sub>O<sub>12</sub> Solid State Electrolyte to Mitigate Li Dendrite Propagation** Asma Sharafi; University of Michigan, United States.

**9:15 AM ES6.10.03**  
**“Dendrites” in Lithium Solid Electrolytes?** Lukas Porz<sup>1,3</sup>; <sup>1</sup>Massachusetts Institute of Technology, United States; <sup>2</sup>Technische Universität Darmstadt, Germany.

**9:30 AM ES6.10.04**  
**Determining Viscoplastic Properties of Lithium Metal by Nanoindentation** Yikai Wang; University of Kentucky, United States.

**9:45 AM ES6.10.05**  
**Silica-Based Organic-Inorganic Hybrid Materials for All-Solid-State Battery Electrolyte Application** Weimin Wang; University of Michigan, United States.

**10:00 AM BREAK**

SESSION ES6.11: Batteries  
Session Chairs: Perla Balbuena and Jianlin Li  
Thursday Morning, April 20, 2017  
PCC North, 200 Level, Room 228 A

**10:30 AM ES6.11.01**

**Mechanics of Battery and Catalysis Materials** Yi Cui; Stanford University, United States.

**10:45 AM \*ES6.11.02**

**Needs and Challenges Associated with High Energy Batteries with an Emphasis on Thermodynamic Underpinnings** Mark Verbrugge; General Motors, United States.

**11:15 AM ES6.11.03**

**Coupling *In Situ* TEM and Ex Situ Analysis to Understand Heterogeneous Sodiotion of Antimony** David Mitlin; Clarkson University, Canada.

**11:30 AM ES6.11.04**

**Measurements of Stress and Fracture in Germanium Electrodes of Li-Ion Batteries** Matt Pharr; Texas A&M, United States.

**11:45 AM ES6.11.05**

**Stress Induced Ionic Interplay in Lithium Sulfur Battery Electrodes** Aashutosh Mistry; Texas A&M University, United States.

SESSION ES6.12: Modeling and Diagnostics in Batteries  
Session Chairs: Jianlin Li and Kejie Zhao  
Thursday Afternoon, April 20, 2017  
PCC North, 200 Level, Room 228 A

**1:30 PM \*ES6.12.01**

**Nanoscale Structural Dynamics in Lithium Ion Batteries Measured by Coherent X-Rays** Y. Shirley Meng; University of California, San Diego, United States.

**2:00 PM ES6.12.02**

**Design and *In Situ* Lithiation of Mechanically Robust, Nano-Architected Battery Electrodes** Xiaoxing Xia; California Institute of Technology, United States.

**2:15 PM \*ES6.12.03**

**A First Principles Comparative Study of Lithium, Sodium and Magnesium Storage in Pure and Gallium-Doped Germanium—Competition between Interstitial and Substitutional Sites** Sergei Manzhos; National University of Singapore, Singapore.

**2:45 PM ES6.12.04**

**First-Principle Density Functional Theory (DFT) Calculations for Screening Functional Additives in High-Voltage Lithium Ion Batteries** Chia-Jung Lee; National Cheng Kung University, Taiwan.

**3:00 PM BREAK**

**3:30 PM \*ES6.12.05**

**Predicting Mechanical Stresses in Lithium-Ion Battery Electrodes Using Mesoscale Simulations** Scott A. Roberts; Sandia National Laboratories, United States.

**4:00 PM ES6.12.06**

**The Densification of Sulfur and Silicon Electrodes for Lithium-Ion Battery Large Scale Production** Jeffrey M. Bell; University of California Riverside, United States.

**4:15 PM \*ES6.12.07**

**Coupled Electrochemical-Mechanical Modeling and Simulation of Lithium-Ion Batteries** Arnulf Latz<sup>1,2,3</sup>; <sup>1</sup>German Aerospace Center, Germany; <sup>2</sup>Helmholtz Institute Ulm, Germany; <sup>3</sup>University of Ulm, Germany.

**4:45 PM ES6.12.08**

***In Situ* TEM Experiments and First-Principles Studies on the Electrochemical and Mechanical Behaviors of  $\alpha$ -MoO<sub>3</sub> in Li-Ion Batteries** Yonghe Li; Beijing University of Technology, China.