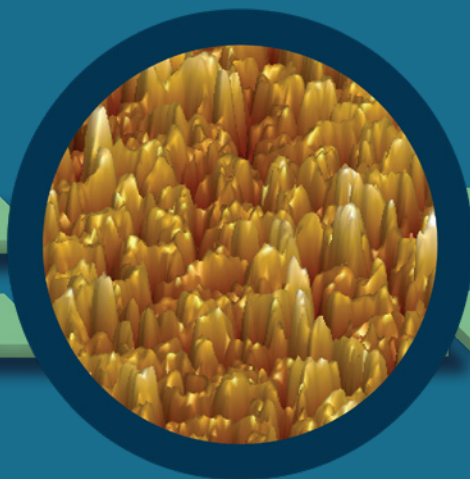


**BOSTON  
UNIVERSITY**

# MATERIALS DAY

**MATERIALS FOR ELECTROCHEMICAL  
ENERGY CONVERSION & STORAGE**



**BU.EDU/ENG/MATERIALSDAY2018**

**BOSTON UNIVERSITY**

Friday, October 26, 2018

Photonics Center, Room 906

8 Saint Mary's Street, Boston MA

AFM image: Yu, Y., Surface segregation in strontium doped lanthanum cobalt ferrite: effect of composition, strain and atmospheric carbon dioxide (Doctoral dissertation), Boston University, 2016.

### **NOVEL MATERIALS FOR ELECTROCHEMICAL ENERGY CONVERSION AND STORAGE: EMERGING OPPORTUNITIES AND CHALLENGES**

As concerns of greenhouse gas emissions and climate change mount, humanity is being forced to address its impact on the environment. In the field of stationary power generation, there is an acute need for grid-based and distributed energy conversion and storage technologies to accommodate increasing off-peak generation of renewable energy.

Critical advancements must be made in the areas of grid storage capacity and fuel-adaptable distributed-energy generation. In the transportation sector alone there is an urgent need for carbon-neutral technologies that deliver higher energy and power densities, longer drive distances and longer lifetimes, and faster recharge times.

A plethora of high-efficiency devices and systems are being considered to

meet these challenges including fuel cells, high temperature electrolyzers, novel batteries, and supercapacitors. Central to the functioning of these devices is the interplay of structure, interphases, charge transfer at electrochemical interfaces, and the transport of charge and mass in response to electrochemical driving forces. The pursuit of long lifetime and reliability hinges on understanding time-dependent phenomena at electrodes and electrolytes that occur at various length scales.

The event will feature top scientists and technologists in the field of electrochemical and energy conversion and storage. It will cover leading edge research on the discovery and synthesis of the materials, structures, architectures, in addition to design strategies.

#### **WORKSHOP ORGANIZER SRIKANTH GOPALAN**

Associate Professor of  
Mechanical Engineering &  
Materials Science and Engineering

## AGENDA

**8:15 AM    REGISTRATION AND CONTINENTAL BREAKFAST**

East End Lounge

**8:45 AM    WELCOME** | Kenneth Lutchen, Dean, College of Engineering and  
Gloria Waters, Vice President and Associate Provost for Research

**9:00 AM    ARUMUGAM MANTHIRAM, UNIVERSITY OF TEXAS**

Electrical Energy Storage: Materials Challenges and Prospects

**9:45 AM    EMILY RYAN, BOSTON UNIVERSITY**

Interfacial Mesoscopic Phenomena in Electrochemical Systems

**10:30 AM    COFFEE BREAK**

East End Lounge

**10:45 AM    SCOTT BARNETT, NORTHWESTERN UNIVERSITY**

High-Efficiency Electrical Energy Storage Using Reversible Solid Oxide Cells

**11:30 AM    WILLIAM WOODFORD, FORM ENERGY**

Long Duration Energy Storage: Opportunities and Challenges  
Introduction: Jacqueline Ashmore, Executive Director, Institute of Sustainable Energy

**12:15 PM    LUNCH BUFFET**

East End Lounge

**1:15 PM    MEILIN LIU, GEORGIA INSTITUTE OF TECHNOLOGY**

Design and Characterization of Electrode Materials for  
High-Performance Supercapacitors

**2:00 PM    LINCOLN MIARA, SAMSUNG RESEARCH AMERICA**

Transitioning to Tomorrow's Batteries: The Solid State Battery

**2:45 PM    COFFEE BREAK**

East End Lounge

**3:00 PM    HARRY TULLER, MASSACHUSETTS INSTITUTE OF TECHNOLOGY**

Engineering Electrochemical Nanoscale Oxides

**3:45 PM    CLOSING REMARKS** | Srikanth Gopalan, Boston University

**4-5:30 PM    POSTER SESSION | WINE & CHEESE RECEPTION**

7<sup>th</sup> Floor Atrium

### SCOTT BARNETT

NORTHWESTERN UNIVERSITY  
PROFESSOR OF MATERIALS SCIENCE  
AND ENGINEERING

#### HIGH-EFFICIENCY ELECTRICAL ENERGY STORAGE USING REVERSIBLE SOLID OXIDE CELLS



**ABSTRACT:** Electrical energy storage is a key technology needed for enabling increased utilization of renewable wind and solar energy resources. While many technologies are being considered, the grid “load shifting” application – storing excess electricity for several hours until there is demand – remains challenging. This presentation will discuss the use of reversible solid oxide fuel cells for grid-scale energy storage. Fuel cells can provide large energy storage capacities by using large storage tanks/caverns for product gases, but until recently have not been strongly considered because of low round-trip efficiency. A new method for improving efficiency will be described, utilizing a new storage chemistry where the fuel cycles between H<sub>2</sub>O-CO<sub>2</sub>-rich and CH<sub>4</sub>-rich gases, allowing much-improved round-trip efficiency > 70%. For this application, however, improved solid oxide cells are needed that can provide useful current densities at relatively low overpotentials and ~ 600oC. A candidate being developed in the Barnett group, utilizing doped lanthanum gallate electrolytes, will be described. Results on the stability of solid oxide cells under thousands of current-switching cycles, a key question that has not previously been explored, will be presented.

**BIO:** Scott A. Barnett is a professor in the Department of Materials Science and Engineering at Northwestern University. His research utilizes physical vapor and colloidal deposition methods for producing ceramic materials with energy applications, including Li-ion battery electrodes and solid oxide fuel cells. Focus areas include three-dimensional tomography of electrode microstructure for understanding electrochemical processes and degradation phenomena, SOFC operation with hydrocarbon fuels, reversible solid oxide cells for energy storage, and development of new fuel cell anode and cathode materials.

## MEILIN LIU

GEORGIA INSTITUTE OF TECHNOLOGY  
REGENTS PROFESSOR OF MATERIALS  
SCIENCE AND ENGINEERING

### DESIGN AND CHARACTERIZATION OF ELECTRODE MATERIALS FOR HIGH- PERFORMANCE SUPERCAPACITORS



**ABSTRACT:** The ever-increasing demand for clean and secure energy has stimulated an intense search for efficient electrical energy storage systems of high energy and power density. For now and in the foreseeable future, supercapacitors represent one of the most attractive options for a diverse range of applications that require rapid power delivery and recharging, from portable electronic devices to electric vehicles and smart grids. However, the performances of the state-of-the-art supercapacitors are still inadequate for many intended applications. The development of a new generation of high-performance supercapacitors depends on the creation of novel electrode materials and structures that may dramatically accelerate the rate of mass and charge transfer processes associated with electrical energy storage. In this presentation, recent progress will be highlighted in investigations into the charge storage mechanisms of promising electrode materials using in situ and operando Raman spectroscopy and density functional theory (DFT)-based calculations. Fundamental understanding of the mechanisms is vital to achieving knowledge-based design of more efficient electrode materials. Perspectives for a new generation of hybrid supercapacitors will also be discussed.

**BIO:** Meilin Liu is the B. Mifflin Hood Chair, Regents Professor, and Associate Chair of the School of Materials Science and Engineering at Georgia Institute of Technology. He received his MS and PhD from University of California at Berkeley. His research interests include design, fabrication, in situ characterization, and modeling of membranes, thin films, coatings, porous electrodes, and devices for electrochemical energy storage and conversion, aiming at achieving rational design of novel materials and structures with unique functionalities. Dr. Liu holds 27 U.S. patents, co-organized 11 international symposia or workshops, co-edited 7 proceedings volumes, delivered ~180 invited lectures around the world, and published ~450 refereed articles. His publications have been cited over 33,000 times in Google Scholar with an h-index of 95. Dr. Liu is a fellow of the American Ceramic Society (ACerS) and the Electrochemical Society (ECS). He is the winner of many professional awards, including HTM Outstanding Achievement Award (ECS, 2018), Charles Hatchett Award (UK IOM3, 2018), Outstanding Faculty Research Author Award (Georgia Tech, 2013 and 1997), Ross Coffin Purdy Award (ACerS, 2010), Outstanding Achievement in Research Program Development Award (Georgia Tech, 2003), Sustained Research Award (Sigma Xi, 2003), and NSF Young Investigator Award (NSF, 1993).

### ARUMUGAM MANTHIRAM

UNIVERSITY OF TEXAS AT AUSTIN  
MATERIALS SCIENCE AND  
ENGINEERING PROGRAM DIRECTOR,  
COCKRELL FAMILY REGENTS CHAIR  
IN ENGINEERING, AND PROFESSOR

#### ELECTRICAL ENERGY STORAGE: MATERIALS CHALLENGES AND PROSPECTS



**ABSTRACT:** Rapid increase in global energy use and growing environmental concerns have prompted the development of clean, sustainable, alternative energy technologies. Electrical energy storage (EES) is critical to efficiently utilize electricity produced from intermittent, renewable sources like solar and wind as well as to electrify the transportation sector. Rechargeable batteries are prime candidates for EES, but their widespread adoption for electric vehicles and grid storage requires optimization of cost, cycle life, safety, energy density, power density, and environmental impact, all of which are directly linked to severe materials challenges. After providing a brief account of the current status, this presentation will focus on the development of advanced materials and new cell chemistries for next-generation battery technologies. Particularly, the challenges and approaches of transitioning from the current insertion-compound electrodes in lithium-ion batteries to new conversion-reaction electrodes with multi-electron transfer to increase the energy density and lower the cost will be presented. Specifically, battery technologies based on lithium and sodium as working ions with high-nickel layered

**BIO:** Arumugam Manthiram is the Cockrell Family Regents Chair in Engineering and Director of the Texas Materials Institute and the Materials Science and Engineering Program at the University of Texas at Austin (UT-Austin). He received his Ph.D. degree in chemistry from the Indian Institute of Technology Madras in 1981. After working as a postdoctoral researcher at the University of Oxford and UT-Austin, he became a faculty member in the Department of Mechanical Engineering at UT-Austin in 1991. Dr. Manthiram's research is focused on rechargeable batteries, fuel cells, and supercapacitors. He has authored more than 700 journal articles with 47,000 citations and an h-index of 110. He is a Fellow of six professional societies: Materials Research Society, Electrochemical Society, American Ceramic Society, Royal Society of Chemistry, American Association for the Advancement of Science, and World Academy of Materials and Manufacturing Engineering. He received the university-wide Outstanding Graduate Teaching Award in 2012, Battery Division Research Award of the Electrochemical Society in 2014, Distinguished Alumnus Award of the Indian Institute of Technology Madras in 2015, Billy and Claude R. Hocott Distinguished Centennial Engineering Research Award in 2016, and Da Vinci Award in 2017. He is a Web of Science Highly Cited Researcher in 2017.

## LINCOLN MIARA

**SAMSUNG RESEARCH AMERICA  
SENIOR STAFF ENGINEER**

### **TRANSITIONING TO TOMORROW'S BATTERIES: THE SOLID STATE BATTERY**



**ABSTRACT:** Solid-state batteries (SSBs) are poised to become the next-generation secondary batteries because of advantages of enhanced safety, thermal stability, and energy density. The journey from concept to commercialization, although not complete, has required much attention to seemingly small details and some creative solutions. This talk will focus on the key computational tools we invented and utilized to accelerate the development of solid state batteries, including new materials discovery and the improved design of interfaces. This talk will also highlight the necessity of close collaboration between academics and industry and between diverse research groups involved in computation, experimentation, characterization, and scale-up; all of which are necessary for the practical realization of new battery technologies.

**BIO:** Dr. Miara has been an engineer with Samsung Electronics for more than 7 years. Prior to that, he earned his PhD from the Boston University Division of Materials Science & Engineering. In addition to working at Samsung, he also worked as an Adjunct Professor at Boston University for several years. Dr. Miara has expertise in ceramic processing, theoretical modeling, and solid state ionics. His work is devoted to the realization of a future powered by carbon free energy sources enabled by electrochemical energy storage and conversion technologies such as batteries and fuel cells suitable for electric vehicles and grid level storage. During his time at Samsung, his work has focused on a range of next generation battery technologies with a particular emphasis on developing and applying atomistic computational tools to overcome major challenges preventing the commercialization of new battery types. This work has expanded into a multi-national collaboration of industry and academic partners. In 2015 he established the Samsung Advanced Materials Laboratory housed in the Boston University Chemistry Department which focuses on the testing of advanced lithium ion battery components.



### EMILY RYAN

**BOSTON UNIVERSITY**  
**ASSISTANT PROFESSOR OF**  
**MECHANICAL ENGINEERING &**  
**MATERIALS SCIENCE AND**  
**ENGINEERING**

#### **INTERFACIAL MESOSCOPIC** **PHENOMENA IN ELECTROCHEMICAL** **SYSTEMS**



**ABSTRACT:** Complex chemical-physical phenomena, such as reactive transport, heat transfer and hydrodynamics, are critical to the operation and performance of advanced electrochemical systems. The critical physics of these systems occurs at the meso-scale interfaces between phases, such as the electrode-electrolyte interfaces in batteries and fuel cells. Experimentally visualizing interfaces is challenging due to their small scales, imbedded nature and complex geometry. Computational modeling is a powerful tool for understanding the physics within these energy systems, especially at interfaces. In this talk I will discuss research into the development of computational methods for the simulation the electrode-electrolyte interface of lithium batteries for the study of dendritic growth. This research focuses on understanding the fundamental driving forces for dendrite growth and exploring strategies for suppressing dendrite growth, including the use of novel electrolyte materials and structural designs.

**BIO:** Professor Emily Ryan is an Assistant Professor in the Department of Mechanical Engineering and the Division of Materials Science and Engineering at Boston University. She received her Ph.D. in mechanical engineering from Carnegie Mellon University in 2009, where her dissertation research focused on numerical modeling of solid oxide fuel cells. After graduating from Carnegie Mellon she worked as a post-doctoral research associate and staff computational scientist in the Computational Mathematics and Engineering group at Pacific Northwest National Laboratory. Since joining Boston University in 2012, she founded the Computational Energy Laboratory, which focuses on the development of computational models of advanced energy systems, including batteries, fuel cells, carbon capture technologies, and fuel injectors. Her research is funded through the National Science Foundation, the Department of Energy and industry.



## HARRY TULLER

MASSACHUSETTS INSTITUTE OF  
TECHNOLOGY

R.P. SIMMONS PROFESSOR OF  
CERAMICS AND ELECTRONIC  
MATERIALS

ENGINEERING ELECTROCHEMICAL  
NANOSCALE OXIDES



**ABSTRACT:** Oxides are playing an increasing critical role as functional components in the fields of energy conversion/storage, microelectronics, sensors/actuators and catalysis. In turn, their electrical (ionic & electronic), optical, and catalytic properties depend sensitively on their defect structure and oxygen nonstoichiometry, typically frozen in during processing, and rarely well defined. This is particularly true for thin films and nanoparticles/wires, where conventional methods, appropriate to bulk materials, do not apply. In this presentation, we review in-situ optical, electrochemical and dilatometric methods, developed or refined in our laboratory, to monitor, analyze and control nonstoichiometry, defect equilibria, transport and optical properties of oxide thin films and nano-sized particles. Examples will include materials of interest as electrodes in fuel cells, and as components of sensors, catalysts and memory devices.

**BIO:** Harry L. Tuller is R.P. Simmons Professor of Ceramics and Electronic Materials, Department of Materials Science and Engineering at the Massachusetts Institute of Technology, Cambridge, Massachusetts, USA. He received B.S. and M.S. degrees in Electrical Engineering and Eng.Sc.D. in Solid State Science & Engineering from Columbia University; served as Postdoctoral Research Associate; Physics, Technion, Israel, following which he joined the faculty at MIT.

His research focuses on defects, diffusion, and the electrical, electrochemical and optical properties of metal oxides with applications to sensors, fuel cells, MEMS and memristive devices.

He has published over 465 articles, and awarded 33 patents. He is Editor-in-Chief of the Journal of Electroceramics; co-founder of Boston MicroSystems, a pioneer in silicon carbide-based MEMS technology and devices and Former President of the International Society of Solid State Ionics (2015-17).

Selected honors include: Fellow - American Ceramic Society –ACERS- (1984); von Humboldt Award (Germany) (1997-2002); Honorary Doctorate, University Provence, Marseilles (2004); elected to World Academy of Ceramics (2006); Honorary Doctorate, University of Oulu, Finland (2009); Outstanding Achievement Award - The Electrochemical Society (2010); Helmholtz International Fellow Award (Germany) (2013); Fellow - Electrochemical Society (2014); President, International Society of Solid State Ionics (2015-17); Life Senior member IEEE; Distinguished Life Member, American Ceramic Society (2016).

## SPEAKERS

### WILLIAM WOODFORD

FORM ENERGY  
CO-FOUNDER AND CTO

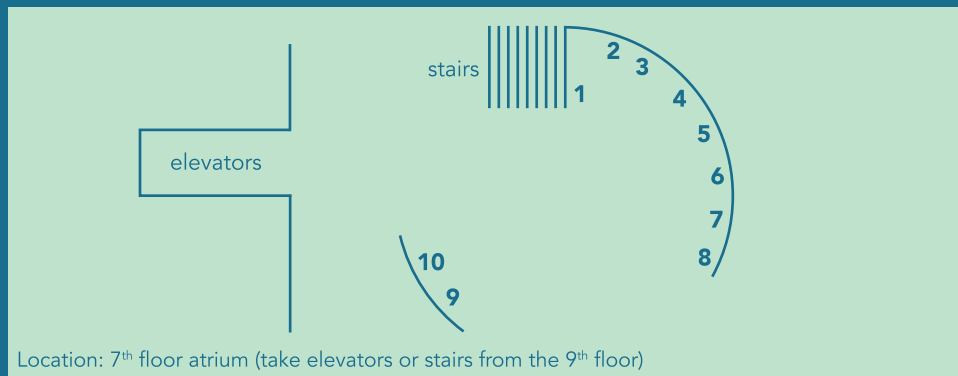
#### LONG DURATION ENERGY STORAGE: OPPORTUNITIES AND CHALLENGES



**ABSTRACT:** Form Energy is developing and commercializing ultra-low cost, long duration energy storage systems that can be located in any market and scaled to match existing energy generation infrastructure globally. These systems have the capability to reshape the electric system, making renewables fully firm and dispatchable year-round. The application whitespace of long duration energy storage opens up new opportunities for electrochemical energy storage systems. This talk will highlight the opportunities and challenges in long duration energy storage.

**BIO:** William Woodford is co-founder and CTO of Form Energy, where he leads the technical team developing low-cost, long-duration energy storage systems to enable a 100% renewable grid. His career has focused on developing robust low-cost energy storage systems based on electrochemical platforms, both in academic and start-up roles. Prior to Form Energy, William was Director of Advanced R&D at 24M Technologies, where his team focused on low-cost automotive and grid storage Li-ion development. In 2018, he was recognized with Technology Review's TR35 award, as one of the top 35 innovators under the age of 35. Dr. Woodford earned his PhD from the Massachusetts Institute of Technology and his BS from the Pennsylvania State University, both in Materials Science and Engineering.

## POSTER SESSION: MAP & TITLES



### POSTER 1

Presenter: Bo Pang  
Institution: BU, MSE  
Advisor: Kevin Smith  
Title: Characterization of Transition Oxide Nano-Particles

### POSTER 2

Presenter: Jennifer Chapman Varela  
Institution: BU, Chemistry  
Advisor: Mark Grinstaff  
Title: Synthesis, Characterization, and Modeling of New Piperidinium Based Ionic Liquid Electrolytes

### POSTER 3

Presenter: Yanchen Lu  
Institution: BU, MSE  
Advisor: Soumendra Basu  
Title: Improving Intermediate Temperature Performance of Ni-YSZ Cermet Anodes for Solid Oxide Fuel Cells by Liquid Infiltration of Nickel Nanoparticles

### POSTER 4

Presenter: Dmitri Kalaev  
Institution: MIT, DMSE  
Advisor: Harry L. Tuller  
Title: Reprogrammable Electro-Chemo-Optical Devices

### POSTER 5

Presenter: Zhikuan Zhu  
Institution: BU, ME  
Advisor: Soumendra Basu  
Title: Electrochemical cleaning: novel, in-situ approach to improving SOFC life time via removal of cathodic chromium deposits

### POSTER 6

Presenter: Paul Gasper  
Institution: BU, MSE  
Advisor: Uday Pal  
Title: Improving electrochemical performance of Nickel-Yttria Stabilized Zirconia anodes employing nickel nanoparticles

### POSTER 7

Presenter: Kunjoong Kim  
Institution: MIT, DMSE  
Advisor: Jennifer Rupp  
Title: Enhanced Charge Transfer at Electrolyte-Electrode Interface for Solid State Li Metal Battery

### POSTER 8

Presenter: Ben Levitas  
Institution: BU, MSE  
Advisor: Srikanth Gopalan  
Title: Core-Shell Heterostructures as Functional Materials for Solid Oxide Fuel Cell (SOFC) Electrodes

### POSTER 9

Presenter: Jane Banner  
Institution: BU, MSE  
Advisor: Srikanth Gopalan  
Title: Rare Earth Nickelate Cathodes for SOFCs in High Oxygen Partial Pressure Environments

### POSTER 10

Presenter: Professor Yu (Michael) Zhong, PhD  
Institution: WPI, ME  
Title: Application of Computational Thermodynamics in Solid Oxide Fuel Cell

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*To access the "Eduroam" network, you must have prior authorization, and your device should be appropriately configured.*

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DEPARTMENT OF MECHANICAL ENGINEERING

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DEPARTMENT OF CHEMISTRY

## MSE PHD STUDENT HOSTS

Paul Gasper, Advised by Uday Pal

Michelle Sugimoto, Advised by Uday Pal

Yanchen Lu, Advised by Soumendra Basu

Ben Levitas, Advised by Srikanth Gopalan

Boshan Mo, Advised by Srikanth Gopalan

Jane Banner, Advised by Srikanth Gopalan

## DIVISION OF MATERIALS SCIENCE AND ENGINEERING STAFF

Elizabeth Flagg, Gabriella McNevin, Ruth Mason

**WORKSHOP ORGANIZER SRIKANTH GOPALAN** would like to express warm gratitude to those who support the organization of Materials Day 2018, and thank all who attend!