2023 Frances S. Sterrett Environmental Chemistry Symposium

What is the Future of Electric Vehicles?

Saturday, November 18, 2023
8:45 a.m. – 3:25 pm
Berliner Hall Room 117
Hofstra University
Hempstead, N.Y. 11549-1000
http://newyorkacs.online/sterrett/

The Frances S. Sterrett Environmental Chemistry Symposium *is committed to delivering current and accurate scientific insights on environmental subjects to the public. Co-hosted by the Long Island Subsection and the New York Section of the American Chemical Society (ACS), this event is made possible with support from the ACS LS-MEET Grant, and Hofstra University's Chemistry Department. We invite you to join us and gain invaluable insights from field experts as they illuminate the path forward for electric vehicles (EVs), exploring the evolution of EV batteries and beyond.*

ACS Chemistry for Life®

ACS Local Section New York Long Island Subsection

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Registration (free): using the link 2023 LIACS-ECS
Contact: Dr. Paris Svoronos – Symposium Chairperson

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8:45 am	**Continental Breakfast**
9:25 am	**Welcome Remarks** Dr. Paris Svoronos, *Symposium Chairperson* Dr. William Nirode, *Chair, Chemistry Department, Hofstra University* Dr. Charles Riordan, *Provost and Senior Vice President for Academic Affairs, Hofstra University* Dr. Mary Virginia Orna, *2023 ACS-NY Chairperson* Dr. Terrence Black, *2023 ACS-LI Chairperson*
9:40 am	**Structural & Dynamical Insights of Novel Li^+ Battery Solid Electrolytes via NMR** Dr. Steve Greenbaum, *CUNY Distinguished Professor, Physics Department, CUNY-Hunter College*
10:10 am	**From Gasoline to Green: Adventures in Old-Fashioned and Electric Car Driving** Dr. Brian Gibney, *Professor & Chair, Department of Chemistry & Biochemistry, Brooklyn College*
10:40 am	**Break**
10:50 am	**Electrolyte Additives & Solvent Development for Li-Metal Batteries** Dr. Muhammad Mominur Rahman, *Chemistry Research Associate, Brookhaven National Laboratory*
11:20 am	**Impact of Repeated Fast Charge on Electric Vehicle Batteries** Dr. Esther Takeuchi, *SUNY Dist. Prof., Knapp Chair in Energy & Environ., Stony Brook University*
11:50 pm	**Lunch Break**
12:30 pm	**New Materials Concepts for Next Generation Electric Vehicle Batteries** Dr. Kenneth Takeuchi, *Distinguished Teaching Prof., Chemistry Department, Stony Brook University*
1:00 pm	**Future Electric Vehicle Batteries: Challenges and Opportunities** Dr. Amy Marschilok, *Energy Storage/System Division Manager, Brookhaven National Laboratory*
1:30 pm	**Break**
1:40 pm	**Multi-electron Redox for Na-ion Battery** Dr. Hao Liu, *Assistant Professor, Chemistry Department, Binghamton University*
2:10 pm	**Prospects of Solid-State Batteries for Electric Vehicles and Beyond** Dr. Priyanka Bhattacharya & Dr. Kevin Wujcik, *Battery R&D, Blue Current*
2:40 pm	**Lithium-ion Battery Materials Consideration Beyond Performance** Dr. Linda L. Gaines, *Transportation Systems Analyst, Argonne National Laboratory*
3:10 pm	**Undergraduate Student Raffle & Closing Remarks** Dr. Ping Furlan, *2024 ACS-NY Chair-Elect* Dr. Sujun Wei, *2023 ACS-LI Chair-Elect*

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Dr. Steve Greenbaum

Structural and Dynamical Insights of Novel Li^+ Battery Solid Electrolytes by NMR Spectroscopy

Steve Greenbaum, Ph.D., CUNY Distinguished Professor

Physics Department, Hunter College of the City University of New York, USA

The successful development of all-solid-state-batteries (ASSB) is critically dependent on solid electrolytes that meet conductivity and mechanical/electrochemical interfacial stability requirements. We present here the results of two recent collaborative efforts. The first one concerns cellulose nanofibers (CNF) derived from natural wood materials. A new strategy has been established via introducing Cu^{2+} into the CNF to achieve a greater mobility of Li^+ ions, where Cu^{2+} opens up one-dimensional nanofibrils and creates molecular channels. Nuclear Magnetic Resonance (NMR) plays a significant role in providing new insights into the structure and dynamics of Li-Cu-CNF materials. Fast magic angle spinning (MAS) ^1H NMR provides estimates of the residual carbonate solvent/H_2O present in Li-Cu-CNF materials, which aids the Li^+ transport mechanism without compromising electrochemical stability. Pulsed Field Gradient (PFG) NMR has been used to measure the diffusivity of Li^+ and anion and to estimate the Li+ transference number t(Li+), which turns out to be significantly greater as compared to the other polymer-based electrolytes. Additionally, the anisotropic diffusion of Li+ and anion in aligned cellulose wood materials have been demonstrated through PFG NMR. Lastly, the local structure of cellulose fibers and their spatial interactions with ionic species are probed through multi-dimensional (1D and 2D) solid state NMR detecting ^1H, ^7Li, ^{19}F, ^{13}C nuclei. Next, we have investigated the novel inorganic solid electrolyte Li_3YCl_6, through a combination of static, MAS, and PFG NMR. Significant effects of milling and thermal treatment on both long- and short-range structural order and on restricted diffusion are observed. A third topic concerns the challenges inherent in forming composites of inorganic ion conductor and polymer. Strategies to produce a material with the "best of both worlds", that is high conductivity and thin film processability, generally have proven to be elusive. We will give several recent examples of (partial) successes and failures.

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Dr. Brian Gibney

From Gasoline to Green: Adventures in Old-Fashioned and Electric Car Driving

Brian R. Gibney, Ph.D., Professor
Department of Chemistry and Biochemistry
Brooklyn College of the City University of New York, USA

The development battery electric vehicles and plug-in hybrids based on advanced battery technology present the consumer with a significant new variable when purchasing a car. The consumer must now evaluate the type of fuel (electric, gas-electric, hydrogen) used by the car along with its local and long-range availability. In this talk, an owner of both an internal combustion engine (ICE) and a battery electric vehicle (BEV) will discuss various aspects of ownership including: fueling, the driving experience, maintenance, repairs and overall cost. The issue of range-anxiety will be discussed along with at-home fueling and engine efficiency. In addition, an evaluation of how 'green' BEVs are will be presented.

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Dr. Muhammad Mominur Rahman

Electrolyte additives and solvent development for Li-metal batteries

Muhammad Mominur Rahman, Ph.D.
Chemistry research associate, Brookhaven National Laboratory

Li-metal batteries (LMB) are widely regarded as the next generation of energy storage devices because they provide energy density almost double that of commercial Li-ion batteries. However, these batteries face the grand challenge of identifying good electrolytes for cycling. Common electrolytes are either only stable against lithium metal anode or against $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC) cathode. Ether electrolytes, for example, offer stable cyclability against Li metal anode but are highly reactive with NMC cathode. In the first part of the presentation, we discuss engineering the electrode-electrolyte interphase of ether-based electrolytes through utilizing interphase forming additives, which significantly enhances electrolyte stability. In the second part of the presentation, we introduce design principles for electrolyte solvents that are simultaneously stable against both electrodes. Significant research effort has been devoted to increasing the cathode stability of common ether electrolytes. In comparison, there is much less effort trying to increase the anode stability of electrolytes that are stable against NMC cathode. One such example is the sulfone solvent. It is attractive due to its good cathode stability but is hindered from practical application because of (1) high viscosity and poor wetting capability and (2) poor anode stability. Here, we solve these issues by modifying the sulfone molecules using resonance and electron withdrawing effect. The viscosity is significantly reduced by delocalizing the electrons through introducing additional oxygen on the molecular backbone and applying appropriate fluorination. Such modifications of the sulfone molecules allow stable cycling of LMBs under commercially relevant conditions.

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Dr. Esther S. Takeuchi

Impact of Repeated Fast Charge on Electric Vehicle Batteries

Esther S. Takeuchi, Ph.D.
William and Jane Knapp Chair in Energy and the Environment
SUNY Distinguished Professor
National Academy of Engineering, Materials Science & Chemical Engineering, Chemistry
Director, Center for Mesoscale Transport Properties (m2M#S)
Stony Brook University, Energy Sciences Directorate, Brookhaven National Laboratory

Lithium-ion battery technology is desirable for electric vehicles (EVs) due to its high voltage, small size, and light weight. These batteries are the dominant power source used in electric vehicles. In addition to high energy density, fast charge capability is desired to facilitate broader consumer adoption and ease the constraints of charging infrastructure. Notably, lithium ion battery capacity retention after many cycles can be compromised by repeated use of fast charge where the drive time of the battery decreases. This presentation will comment on some of the degradation modes that take place under repeated fast charge and mitigation strategies that could be implemented to extend battery lifetime under these use conditions.

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Dr. Kenneth J. Takeuchi

New Materials Concepts for Next Generation Electric Vehicle Batteries Dr. Kenneth J. Takeuchi, Ph.D.
Distinguished Teaching Professor, Chemistry Department
Stony Brook University

Transportation is the single largest contributor to direct emissions in the US energy system according to a recent National Academy report. Thus, movement toward low or zero emissions cars is an important step toward lowering overall emissions where electrification of vehicles plays a pivotal role in achieving decarbonization goals. Currently, lithium ion batteries are the dominant power source for electric vehicles. Yet, challenges remain for broadening use of electric vehicles including batteries that are large and heavy. Alternative reaction modalities beyond simple ion insertion can provide higher energy content resulting in higher energy output batteries. Next generation battery concepts that are smaller and lighter potentially enabled by new materials design approaches will be discussed in this presentation.

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Dr. Amy Marschilock

Future Electric Vehicle Batteries: Challenges and Opportunities

Amy Marschilock, Ph.D.
Co-Director, Institute of Energy: Sustainability, Environment, and Equity (I:SEE)
Professor, Department of Chemistry
Adjunct Faculty, Materials Science and Chemical Engineering
Stony Brook University 675 Chemistry

The Unique Behavior of 2-Dimensional Materials: Role in Batteries for Electric Vehicles

The expansion of electric vehicle adoption can be impacted by the cost and availability of the raw materials used in the batteries that power them. Currently, some of the materials used in batteries powering electric vehicles are available only in limited areas in the world, are rare and thus, expensive. It would be advantageous to construct batteries based on low-cost abundant materials available over a wide geographic range. One example of a material of high interest for lithium batteries is sulfur due to its low cost and high theoretical capacity. However, the implementation of the system has been challenged due to the instability of the batteries and their degradation under use. Our research has shown that the use of 2D materials can offer significant benefit to batteries and provide new design approaches for next generation batteries.

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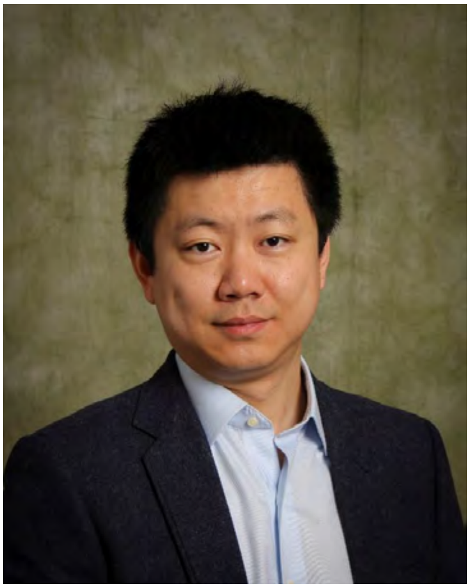

Dr. Hao Liu

Multi-electron redox for Na-ion batteries

Hao Liu, Ph.D., Assistant Professor
Department of Chemistry,
Binghamton University

The charge storage capacity of battery cathode materials is governed by the number of electrons transferred per redox center. Most intercalation-based electrodes are based on one-electron transfer per transition metal ion center, which limits their theoretical capacity. Enabling multi-electron transfer per transition metal ion center could potentially multiply the charge storage capacity of electrode materials. While intercalation compounds with multielectron redox have been demonstrated for Li-ion batteries, few cases have been reported for Na-ion batteries. We have explored a couple of silicate- and phosphate-based materials for their activity for multi-electron redox. A multitude of structural, spectroscopic, and electrochemical methods were used to elucidate their reaction mechanisms. The intercalation of the larger Na ions induces substantial structural rearrangement to accommodate the multi-electron redox reaction, yet the reversibility of such reaction is greatly compromised, undermining their application in practical batteries.

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Dr. Kevin Wujcik

Dr. Priyanka Bhattacharya

Prospects of Solid-State Batteries for Electric Vehicles and Beyond

Priyanka Bhattacharya, Ph.D. – Sr. Manager, Battery R&D, Blue Current
Kevin Wujcik, Ph.D. – Chief Technology Officer, Blue Current

Solid state batteries have reached a point of technological maturity beyond academic labs and are being considered for commercialization by several manufacturers throughout the world. For a scaled production, four key challenges need to be addressed – high safety, low operating pressure, wide range of operating temperatures, and scalability. Blue Current manufactures 100% dry, safe and high-performance silicon elastic composite solid-state batteries to power the new energy economy including electric vehicles and non-automotive applications. The company is building its first Megawatt-scale pilot factory in California that will produce sample batteries for industry partners and customer validation. We see the potential for a new silicon elastic composite battery that's highly resistant to fire, provides high energy density, remarkable cycle life at low operating pressures, and room temperature operation, thus making it a scalable and viable solid-state battery. Chemistry is the hardest part of battery development. Getting the chemistry right first provides a better chance of scaling successfully, particularly using existing high volume manufacturing systems. In this presentation, we will address the above key challenges and Blue Current's solutions that encompass improving the fundamental properties of 100% solid cathode, anode and separator.

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Dr. Linda Gaines

Material Supply Considerations for Lithium-Ion Batteries

Linda Gaines, Ph.D.
Transportation System Analyst
Argonne National Laboratory

Rapid growth of lithium-ion battery use is projected to continue in the transportation sector, leading to concomitant growth in demand for the constituent materials. But experts foresee imminent shortages in key materials, such as lithium, nickel, and cobalt. To what extent can recycling alleviate these looming supply constraints? What other materials can be used if key material supplies prove insufficient or too expensive? How can other technological options enable the US to supply continued mobility for both people and the goods they require? This presentation will provide insights into the answers to these questions.

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Special Thanks to

The Symposium Committee Members

Dr. Paris Svoronos, Chair
Dr. Kevin Bisceglia
Dr. Terrence Black
Dr. Ronald P. D'Amelia
Dr. Ping Furlan
Dr. Brian Gibney
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