Joint APS/CNM Workshop 5: Emerging Opportunities for Battery Research and Manufacturing: Data-driven Multiscale/Multimodal Analysis

Tuesday, May 6, Afternoon

1:30 – 1:40 Workshop Organizers
Welcome and Opening Remarks

1:40 – 2:10 Tanvir Tanim (Idaho National Laboratory)
Accelerating Battery Innovation: Integrating Advanced Data Science and Characterization Techniques for Rapid Validation and Failure Mode Understanding

2:10 – 2:40 Susan Babinec (Argonne National Laboratory)
Rapid and Accurate Life Prediction: A Transformational Capability

2:40 – 3:10 Jordi Cabana (Argonne National Laboratory and University of Chicago)
Quantification of Chemical Heterogeneity in Battery Cathodes: Where Should We Look?

3:10 – 3:20 Break

3:20 – 4:20 Ashfia Huq (Molecular Foundry, Lawrence Berkeley National Laboratory)
Carlo Segre (Advanced Photon Source, Argonne National Laboratory), and
Tao Zhou (Center for Nanoscale Materials, Argonne National Laboratory)
Data-based Science-driven Battery Research and Manufacturing at DOE User Facilities

4:20 – 5:30 Chibueze Amanchukwu (University of Chicago), Susan Babinec (Argonne National Laboratory), Jordi Cabana (Argonne National Laboratory and University of Chicago), Ashfia Huq (Lawrence Berkeley National Laboratory), and Tanvir Tanim (Idaho National Laboratory)
Panel Discussion: Needs and Opportunities for Data-driven Battery Research

5:30 Adjourn Day One

Wednesday, May 7, Afternoon

1:30 – 1:40 Workshop Organizers
Welcome and Opening Remarks

1:40 – 2:10 Arumugam Manthiram (Walker Department of Mechanical Engineering, University of Texas at Austin)
Emerging Opportunities with Cathodes for Energy Storage

2:10 – 2:40 Jay Whitacre (Carnegie Mellon University and Stratus Materials Inc.)
Scaled Production of Next Generation Lithium/Manganese-rich Cathode Materials: The Promise of Novel Processes and Characterization Methods

2:40 – 3:10 Kyeongjae Cho (Department of Materials Science and Engineering and BEACONS Center, University of Texas at Dallas)
Rational Design of Battery Cathode Materials to Battery Cell Prototyping at BEACONS

3:10 – 3:20 Break

3:20 – 3:50 Sili Deng (Department of Mechanical Engineering, Massachusetts Institute of Technology)
Scientific Machine Learning for Inverse Modeling

3:50 – 4:20 Jinyun (Jared) Liao (Princeton NuEnergy Inc.)
Advancing Battery Cathode Manufacturing: Strategies for Cost Reduction and Quality Control

4:20 – 5:30 Neal Dawson-Elli (Nanoramic Inc.), Jeffrey Lopez (Northwestern University), Noah Paulson (Argonne National Laboratory), and Francis Joseph Alexander (Argonne National Laboratory)
Panel Discussion: Needs and Opportunities for Data-driven Battery Manufacturing

5:30 Adjourn

Accelerating Battery Innovation: Integrating Advanced Data Science and Characterization Techniques for Rapid Validation and Failure Mode Understanding

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Batteries are experiencing rapid advancements in both materials selection and emerging use cases. As new options for battery use and design emerge, there is a critical need to validate performance and understand failure modes. Traditionally, validation processes required years of testing and significant resources to achieve acceptable certainty that a new battery would function as intended. However, the recent integration of failure mode analysis with machine learning and advanced data analytics offers the opportunity to dramatically reduce validation time, accelerating the transition from bench-top discoveries to consumer applications.

The rapid validation time has largely relied on time-domain electrochemical data, which has limitations in providing full insights into battery failure mechanisms at the materials and surface/interphase levels—areas critical for remediation. This discussion with example case studies will focus on the needs and opportunities associated with integrating various forms of characterization with advanced data science. By leveraging multimodal methodologies, we can further advance the battery development lifecycle with a comprehensive understanding of failure modes and the mechanisms driving them.

Rapid and Accurate Life Prediction: A Transformational Capability

Susan Babinec[1], Noah Paulson[1], Victor Venturi[1], Vignesh Sampath[1], and Logan Ward

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Life prediction is the key energy storage metric. It provides guidance from discovery research through pilot lines and large-scale manufacturing; it is essential for cost-effective system designs and optimizing performance in the field. Life prediction is a strong function of cell design, cell chemistry, and use case; but unfortunately, it historically is plagued with low accuracy due to the large resources investments and extensive time required for traditional lab evaluations. The data science team of DOE's AI life prediction initiative – ROVI (Rapid Operational Validation Initiative) – has solved this problem using a combination of lab, synthetic, and field data to create world-class tools that can speed life prediction from ~3 years down to ~1 day. This transformative capability not only speeds technology development, but also reduces risks for investors.

Quantification of Chemical Heterogeneity in Battery Cathodes: Where Should We Look?

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[2]Materials Science Division, Argonne National Laboratory, Lemont, IL 60439

The evolution of local chemistry determines the performance of electrodes and electrolytes used in batteries because limitations can be tracked to slow kinetics and transport, and irreversibility in the storage reaction. Tools that provide insight into local chemistry are critical for identifying the underpinnings of electrochemical function. This information must be resolved within architectures, from individual particles to microscale domains, to pinpoint the relationship between local phenomena and their role in macroscopic metrics and degradation. Technical developments in x-ray microscopy and mapping have built a flexible suite of tools that combine the desired spatial resolution and 3D capabilities with a suite of possible contrasts mechanisms, such as diffraction and spectroscopy. In this talk, we will discuss our recent research that demonstrates the diversity of length scales at which important chemical heterogeneity can be induced in battery electrodes, from their synthesis to their operation. For this purpose, the systems of study will be the leading cathodes for Li-ion batteries. We will highlight the new fundamental insight generated by the tools but also showcase the value of continuously seeking to extend analytical capabilities into outcomes of high statistical significance. The insight generated by our approaches will be related to their impact on material and architecture properties. Along the way, we will discuss the prospects of probing time-resolved phenomena using operando measurements to avoid uncertainty due to relaxation under open circuit conditions. We will also provide a glimpse into the future by showing how emerging synchrotron techniques can enhance the impact of x-ray microscopy in fundamental battery science.

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Emerging Opportunities with Cathodes for Energy Storage

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Batteries have become an integral part of our daily life with respect to portable electronic devices. Lithium-ion batteries are dominating the portable devices market due to their high energy density. The battery market is now rapidly expanding with electric vehicles and grid storage of electricity produced from renewable sources. Therefore, as we move forward, cost, sustainability, and supply-chain challenges will be the dominant factor, while maintaining adequate safety.

The fundamental solid-state inorganic chemistry embarked in the 1980s led to the discovery and development of oxide cathodes. They are layered, spinel, and polyanion oxide cathodes. Among them, the layered and polyanion oxide cathodes dominate the commercial lithium-ion battery market. These cathodes will still dominate the field, but with fierce efforts to reduce or eliminate less abundant and expensive metals in the cathode and lower the manufacturing cost. Therefore, this presentation will focus on eliminating or reducing the most expensive cobalt, then the next expensive nickel, and finally eliminating lithium itself with sodium in layered or polyanion oxide cathodes. Opportunities and benefits of blending layered oxides with polyanion oxide cathodes will be discussed. The presentation will articulate the fundamental, intricate roles of electronic configurations and chemical bonding (ionic vs. covalent) on the structural, chemical, air, and thermal instabilities of layered and polyanion oxide cathodes for both lithium-ion and sodium-ion batteries. The importance of cathode manufacturing while reducing liquid chemical waste produced will be emphasized.

Scaled Production of Next Generation Lithium/Manganese-rich Cathode Materials: The Promise of Novel Processes and Characterization Methods

Jay Whitacre[1,2]

[1]Carnegie Mellon University, Pittsburgh, PA 15213
[2]Stratus Materials Inc., Pittsburgh, PA 15208

The lithium-rich/manganese-rich (LMR) class of battery materials has been under investigation for over 25 years and while there has been incremental progress in improving stability and performance, there has been a persistent lack of agreement around the actual structural nature of the material and the source of its unusual functionality and instability. As produced, the material exhibits a dual-phase composition (consisting of segregated nano-domains, or a biphasic solid solution with a crystalline superstructure, depending on synthetic route) and undergoes a significant crystallographic reorganization when delithiated for the first time. Subsequent use typically shows very high specific capacity values (up to 300 mAh/g), but this comes with a rapid collapse in operational potential as the material transforms from the initial layered structure into a spinel structure during electrochemical cycling. A new approach to stymieing this undesirable transition will be disclosed: utilizing an ultra-rapid quench step that locks in an unusually entropic crystallographic state where the transition metal atom organization and the organization of the different phases present in the structure is highly disordered. LMR frozen in this non-equilibrium condition, called LXMO by Stratus Materials, is substantially more functional and stable than traditional LMR materials. Several different scalable processing routes will be discussed, and performance of large format cells based on this material with highly appealing energy densities (over 800 Wh/l) will be disclosed. Additionally, the benefits of several novel/cutting characterization techniques will be reviewed.

Rational Design of Battery Cathode Materials to Battery Cell Prototyping at BEACONS

Kyeongjae (KJ) Cho[1,2]

[1]Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX 75080
[2]BEACONS Center, University of Texas at Dallas, Dallas, TX 75252

Current Li ion batteries (LIBs) are improved versions of the 1991 Sony LIB based on graphite anode, organic liquid electrolytes, and $LiCoO_2$ layered oxide cathode. In the commercial applications of LIBs, cathode materials are known to be the critical component in determining the battery cost (~50% of material cost) and the energy storage capacity (cell capacity = ~1/3 cathode capacity). Over the last 30 years, the initial $LiCoO_2$ cathode (~140 mAh/g charge capacity) has evolved to high capacity cathodes with increasing Ni content replacing Co starting from $Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2$ or NCM111 (~160 mAh/g) to NCM433, NCM532, NCM622, NCM721, NCM811 (~200 mAh/g), and $LiNiO_2$ (> 200 mAh/g). With 70-80% Ni in NCM cathodes (theoretical capacity of ~275 mAh/g), more than 70% of Li can be utilized in the electrochemical reactions in realizing the high-capacity cathode. However, in the fully charged state of LIBs, cathode materials are very unstable toward chemical reactions (irreversible reactions with electrolytes, oxygen evolution and phase changes) and mechanical degradation (interface crack formation). Specifically, the high-Ni NCM cathode materials are known to have large volume change (-7%) at 80% delithiation with the majority of volume change ($\Delta V/V$ = -5%) happening at Li delithiation from 70% to 80% leading to the mechanical cracking of the secondary cathode particles. In this talk, we will discuss multiscale modeling study based on density functional theory (DFT) calculations to examine the atomic and electronic structure origins of the cathode degradation mechanisms [1,2]. Based on the identified microscopic mechanisms at atomic scales, surface and mechanical stabilization methods are designed for experimental validations. The findings in material design research are the basis of current high-throughput robotic synthesis work for the validation experiments. After successfully synthesizing the designed cathode materials, prototype battery cells (18650 and pouch cells) will be produced at the battery R&D line at UTD. University of Texas at Dallas has established the BEACONS center (https://beaconsusa.org/) to strengthen the U.S. energy storage systems industry through an improved domestic supply chain, new battery innovations and a qualified workforce. We will discuss the center facility for R&D line battery production of pouch cells and cylindrical cells (18650, 21700). We will highlight the advanced manufacturing scale-up of battery materials based on AI/ML methods and advanced metrology for accelerated battery manufacturing.

[1] F. Kong, C. Liang, L. Wang, Y. Zheng, S. Perananthan, R. C Longo, J. P Ferraris, M. Kim, K. Cho, "Kinetic Stability of Bulk LiNiO2 and Surface Degradation by Oxygen Evolution in LiNiO2-Based Cathode Materials," Advanced Energy Materials 9 (2), 1802586 (Jan. 10, 2019).
[2] M. Bergschneider, F. Kong, P. Conlin, T. Hwang, SG Doo, K. Cho, "Mechanical Degradation by Anion Redox in $LiNiO_2$ Countered via Pillaring," Adv. Ene. Mater. (Dec. 10, 2024).

Scientific Machine Learning for Inverse Modeling

Sili Deng[1]

[1]Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

This talk introduces two recent scientific machine learning frameworks for inverse modeling in chemically reacting systems. The first framework is a Chemical Reaction Neural Network that integrates physical constraints into its architecture, enabling the autonomous discovery of chemical models from experimental data. This approach has already provided valuable insights into the thermal runaway kinetics of NMC cathode materials. The second framework is a PDE-constrained model parameter calibration method that, for example, leverages thermal wave propagation data to inversely determine transport and reaction properties. This method holds significant promise for advancing our understanding of phase change phenomena and degradation evolution dynamics in battery systems. Together, these frameworks showcase the powerful synergy between machine learning and physics-based modeling, paving the way for more predictive and robust battery performance analysis.

Advancing Battery Cathode Manufacturing: Strategies for Cost Reduction and Quality Control

Jinyun (Jared) Liao[1]

[1]Princeton NuEnergy Inc., Bordentown, NJ 08505

As global demand for lithium-ion batteries continues to surge, improving sustainability, cost efficiency, and quality of battery cathode manufacturing has become a critical challenge. This talk will explore Princeton NuEnergy's (PNE) advanced cathode direct recycling, upcycling, and manufacturing innovations, highlighting strategies to reduce costs while maintaining or enhancing material performance. This presentation will discuss key aspects of cathode material recovery, reprocessing efficiency, and manufacturing optimizations that drive down costs and improve sustainability. We will showcase real-world case studies and performance metrics demonstrating how these innovations contribute to a circular battery economy, reducing dependence on raw material mining and lowering overall production costs.

Princeton NuEnergy (PNE), a U.S.-based innovative clean-tech company, initiated its pilot production in 2022 and manufacturing plant in 2024. PNE is revolutionizing the supply chain of critical materials through its patented technology for directly producing cathode active materials. Utilizing an innovative plasma-assisted process, PNE efficiently produces high quality cathode active materials, making them suitable for direct reintroduction into cell manufacturing. PNE's technology is set to significantly disrupt the battery market, representing a major leap forward in sustainable material recovery and manufacturing.