Program of the **MDB 2025**

Material Development for Batteries (MDB): Progresses and Challenges

Sep. 29 – Oct. 3, 2025

Sejong University, Seoul, South Korea

Organizing Committee

- Conference Co-Chair

- Prof. Dr. Payam Kaghazchi, Forschungszentrum Juelich GmbH, Germany; University of Twente, The Netherland
- Prof. Seung-Taek Myung, Sejong University, South Korea

- Scientific Committee

- Prof. Dr. Payam Kaghazchi, Forschungszentrum Juelich GmbH, Germany; University of Twente, The Netherland
- Prof. Seung-Taek Myung, Sejong University, South Korea
- Prof. Yang Zhao, University of Western Ontario, Canada
- Prof. Javier Carrasco, EnergiGUNE, Spain

Scientific Program

- Alkali-ion batteries (Li-, Na, and K-)
- Alkali metal batteries (Li-, Na, and K-)
- Solid-State-Batteries
- Simulation, Modeling, and Machine learning/AI

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Monday 29 September 2025 – *Morning*

Oral presentation

Room: 1

Chaired by Prof. Seung-Taek Myung

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Sang-Young Lee (Yonsei University, South Korea)
Scalable Electrode Engineering for High-Energy Li Batteries

10:00 – 10:30 **Keynote**
Naoaki Yabuuchi (Yokohama National University, Japan)
Nanostructured Insertion Materials for Practical Li-ion Battery Applications

10:30 – 10:50
Coffee Break

Chaired by Prof. Naoaki Yabuuchi

10:50 – 11:15 **Invited**
Chun-Chen Yang (Ming Chi University of Technology, Taiwan)
Third Generation Ni-rich Cathode Materials: Full-Concentration Gradient FG NCM92 Cathode Materials via a Taylor Flow Reactor

11:15 – 11:40 **Invited**
Jongsoon Kim (Sungkyunkwan University, South Korea)
Development of High-Performance Cathodes for Lower-Cost Alternatives Beyond Conventional LIBs

11:40 – 12:05 **Invited**
Kingo Ariyoshi (Osaka Metropolitan University, Japan)
Solid-State Li-Ion Diffusion in Lithium Insertion Materials Examined by the Diluted Electrode Method

12:05 – 12:30 **Invited**
Jinkwang Hwang (Kyoto University, Japan)
Overlooked Reductive Decomposition Behavior of Ionic Liquid

12:30 – 13:30
Lunch Break (2nd Floor Big Bear Restaurant)

Monday 29 September 2025 – *Afternoon*

Oral presentation

Room: 1

Chaired by Prof. Chun-Chen Yang

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Kyungjung Kwon (Sejong University, South Korea)
Maximizing the doping effect of Al in the resynthesis of NCM cathode active material for Li-ion battery recycling

13:55 – 14:10 **General**
Aktilek Akhmetova (Sejong University, South Korea)
Toward Durable Water-in-Salt Electrolyte Lithium-Ion Batteries Under Practical Conditions

14:10 – 14:40 **Keynote**
Nicolas Bucher (Varta, Germany)
The long road of new materials towards industrialization - a show-case based on Silicon

14:40 – 15:05 **Invited**
Sung-Soo Kim (Chungnam National University, South Korea)
Grain Size Engineering of Porous Si-Alloy Anodes for Enhanced Electrochemical Stability

15:05 – 15:25
Coffee Break

Chaired by Dr. Nicolas Bucher

15:25 – 15:55 **Keynote**
Yuki Yamada (The University of Osaka, Japan)
Electrolyte Li^+ chemical potential dominates graphite anode reactions in lithium-ion batteries

15:55 – 16:20 **Invited**
Jeng-Kuei Chang (National Yang Ming Chiao Tung University, Taiwan)
Ionic Liquid-Based High-Entropy Electrolyte for High-Reliability Lithium-Ion Batteries

16:20 – 16:35 **General**
Bibin Jose (Forschungszentrum Jülich GmbH, Germany)
Ab-initio Insights into Mixed Polyanionic Cathode Materials for Sodium- Ion Batteries

Chaired by Prof. Kyungjung Kwon

16:35 – 16:50 **General**
Dongyoon Kang (Yonsei University, South Korea)
A Tailored Adhesive-Conductive Interlayer for Interface Stabilization of Large-Scale Lithium Metal Powder Electrodes for High-Energy-Density Batteries

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16:50 – 17:05 **General**
Unho Jung (Helmholtz Institute Ulm (HIU), Germany)
Introducing Non-Soluble Additives in Carbonate-based Electrolytes for Lithium-Metal Batteries

17:05 – 17:20 **General**
Konstantin Köster (Forschungszentrum Jülich GmbH, Germany)
Atomistic Configurational Optimizations in Battery Materials: Applications of the GOAC Code

17:20 – 17:35 **General**
Hira-Fatima (Korea Electrotechnology Research Institute (KERI), South Korea)
Adhesion and Surface Engineering of CNT Cathodes by Microwave Treatment for Enhanced Lithium–Sulfur Battery Stability

17:35 – 17:50 **General**
Dijana Milosavljevic (Forschungszentrum Jülich GmbH, Germany)
Design of cathode materials using machine learning and atomistic approaches

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Tuesday 30 September 2025 – *Morning*

Oral presentation

Room: 1
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08:00 – 08:30 **Keynote**
Kazuhiko Matsumoto (Kyoto University, Japan)
Electrolyte Design of Sodium Metal Batteries

08:30 – 08:55 **Invited**
Mario Marinaro (ZSW, Germany)
Enhanced Na-ion Storage: Effect of Elemental Excess and Carbon Coating in $Na_4Fe_3(PO_4)_2(P_2O_7)$

08:55 – 09:20 **Invited**
Wei-Ren Liu (Chung Yuan Christian University, Taiwan)
Nano-crystalline $Fe_3V_3O_8$ Material as an Efficient Advanced Anode for Energy Storage Applications

Chaired by Prof. Kazuhiko Matsumoto

09:20 – 09:45 **Invited**
Masashi Okubo (Waseda University, Japan)
Thermal Stability Index of Sodium Layered Oxide Cathodes

09:45 – 10:10 **Invited**
Changhee Lee (Tokyo University of Science, Japan)
Toward Practical Application of P-Type $Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ Cathodes in Sodium-ion Batteries

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Chaired by Prof. Masashi Okubo

10:30 – 10:55 **Invited**
Aishuak Konarov (Nazarbayev University, Kazakhstan)
Exploring Ni/Fe/Mn-Based Layered Cathodes for Next- Generation Sodium-ion Batteries

10:55 – 11:20 **Invited**
Natalia Voronina (Sejong University, South Korea)
Anionic Redox Chemistry in Layered Sodium Manganese Oxide Cathodes

11:20 – 11:35 **General**
Liang-Ting Wu (National Taiwan University of Science and Technology, Taiwan)
Machine Learning–Driven Phase Stability Prediction for Na-Ion Battery Cathodes

Chaired by Prof. Changhee Lee

11:35 – 12:00 **Invited**
Sebastian Risse (Helmholtz-Zentrum Berlin (HZB), Germany)
From Electrode Breathing to Pressure Mapping: Operando Insights into Sodium Battery Materials

12:00 – 12:25 **Invited**
Jiefang Zhu (Uppsala University, Sweden)
Real-Time Insights: Synchrotron-Based XRD and Tomography for Unveiling Battery Mechanisms

12:25 – 13:25
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Tuesday 30 September 2025 – *Afternoon*

Oral presentation

Room: 1

Chaired by Dr. Sebastian Risse

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Nuclear Magnetic Resonance in Battery Research

13:50 – 14:15 **Invited**
Laura Simonelli (CELLS-ALBA Synchrotron, Spain)
Fostering Battery Innovations by Advanced Synchrotron Techniques: Challenges and Opportunities

14:15 – 14:40 **Invited**
Yong-Min Lee (Yonsei University, South Korea)
Microstructure-resolved Digital Twin Modeling and Simulations for Calendering Process and Dry Electrodes

14:40 – 15:05 **Invited**
Israel Temprano (University of A Coruña, Spain)
Accelerating battery innovation through operando gas analysis

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Chaired by Prof. Aishuak Konarov

15:25 – 15:55 **Keynote**
Zhumabay Bakenov (Nazarbayev University, Kazakhstan)
Development of a Zn/$LiFePO_4$ Aqueous Battery System with $ZnCl_2$/LiCl Binary Electrolyte for Commercial Applications

15:55 – 16:20 **Invited**
Watchareeya Kaveevivitchai (National Cheng Kung University, Taiwan)
Material-Level Engineering of Sustainable Organic Electrode Materials for Ultrahigh-Performance Energy Storage Systems

16:20 – 16:45 **Invited**
Tzu-Ho Wu (National Yunlin University of Science and Technology, Taiwan)
Designing Advanced Cathode Materials for Aqueous Zn-Ion Batteries with High-Rate and High-Areal-Capacity

Chaired by Prof. Natalia Voronina

16:45 – 17:10 **Invited**
Kai Zhu (Harbin Engineering University, China)
Interfacial Design for Zn metal anode towards Aqueous Batteries

17:15 – 17:25 **General**
Lars Winkler (Forschungszentrum Jülich GmbH, Germany)
Zr Incorporation into Lithium Nickel Oxides: Solid Solution or Two-Phase System

17:25 – 18:00
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18:00 – 20:00
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Wednesday 1 October 2025 – *Morning*

Oral presentation

Room: 1

Chaired by Prof. Dr. Payam Kaghazchi

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Bing Joe Hwang (NTUST, Taiwan)
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09:30 – 10:00 **Keynote**
Xiangxin Guo (Qingdao University, China)
Manipulating surface properties of garnet electrolytes for high-rate and long-cycle solid-state lithium batteries

10:00 – 10:30 **Keynote**
Kyung Yoon Chung (Korea Institute of Science and Technology, South Korea)
Research Trends and Cathode Engineering Strategies for High Performance All-Solid-State Lithium–Sulfur Batteries

10:30 – 10:50
Coffee Break

Chaired by Prof. Dr. Kyung Yoon Chung

10:50 – 11:15 **Invited**
Dominic Bresser (Karlsruhe Institute of Technology, Germany)
Single-Ion Polymer Electrolytes based on Polysiloxane for Next-Generation Lithium Batteries

11:15 – 10:40 **Invited**
Sylvain Franger (University Paris-Saclay, France)
Comprehensive study of ionic mobility in hybrid solid-state electrolyte for the next generation of batteries

11:40 – 12:05 **Invited**
Hsisheng Teng (National Cheng Kung University, Taiwan)
Composite Electrolytes for Solid-State Lithium Batteries

12:05 – 12:30 **Invited**

Masashi Kotobuki (Ming Chi University of Technology, Taiwan)
Compatibility of polyimide separator with full cyclic carbonate electrolytes

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Wednesday 1 October 2025 – *Afternoon*

Oral presentation

Room: 1

Chaired by Prof. Dominic Bresser

13:30 – 13:55 **Invited**
Chan-Jin Park (Chonnam National University, South Korea)
3D Porous Single-Ion Conductive Polymer Electrolyte for High-Performance Lithium-Metal Batteries

13:55 – 14:20 **Invited**
Shuai Yuan (Shanghai University, China)
High-performance polymer-based solid-state electrolyte for lithium metal batteries

14:20 – 14:45 **Invited**
Yi-Hung Liu (National Central University, Taiwan)
PVDF/NASICON-Based Composite Solid Electrolytes for Enhanced Sodium-Ion Battery Performance

Chaired by Prof. Bing Joe Hwang

14:45 – 15:10 **Invited**
Ernesto E. Marinero (Purdue University, USA)
Engineering transport properties in polymer composite electrolytes by filler particle additions

15:10 – 15:35 **Invited**
Giuseppe Antonio (Politecnico Di Torino, Italy)
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15:55 – 16:20 **Invited**
Derrick Fam Wen Hui (National University of Singapore, Singapore)
An elastic solution to solid polymer-based Li metal batteries

16:20 – 16:45 **Invited**
Xiaodong Wu (Suzhou Institute of Nano-tech & Nano-bionics, CAS, China)
Preparation and Application of Polymer Solid-State Electrolyte

16:45 – 17:00 **General**
Yixuan Guo (Karlsruhe Institute of Technology (KIT), Germany)
Polysiloxane-Based Single-Ion Conducting Polymer Electrolyte for Na-Metal Batteries

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Mauricio Rincón Bonilla (Basque Center for Applied Mathematics, Spain)
Unsupervised Framework for Automating the Analysis of Structure and Diffusion in Solid-State Electrolytes from Atomistic Simulations

17:25 – 17:50 **Invited**
Jyh-Chiang Jiang (NTUST, Taiwan)
Computational study of Solid Electrolyte Interphase in Lithium Batteries

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Hyungsub Kim (Korea Atomic Energy Research Institute, South Korea)
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Alexandre Tkatchenko (University of Luxembourg, Luxembourg)
Non-local interactions determine local structure and lithium diffusion in solid electrolytes

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Melanie Rosen (FZJ Jülich, Germany)
Materials and Electrode design optimization for oxide based all-solid-state batteries

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Kyung-Wan Nam (Dongkuk University, South Korea)
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10:40 – 11:05 **Invited**
Qianli Ma (FZJ-IMD-2, Germany)
Na^+-ion conducting ceramics with superior performances

11:05 – 11:30 **Invited**
Yongcheng Jin (Ocean University of China, China)
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11:30 – 12:00 **Keynote**
Kee-Sun Sohn (Sejong University, South Korea)
Active Learning for Battery Materials Discovery

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Jose Maria Castillo Robles (DTU, Denmark)
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Thursday 2 October 2025 – *Afternoon*

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Chaired by Dr. Qianli Ma

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Kourosh Malek (FZJ, Germany)
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13:50 – 14:05 **General**
Wen-Qing Li (Institute of High Performance Computing IHPC, Singapore)
Machine-learning-powered molecular dynamics simulations for accurate modelling of SEI materials in lithium-ion batteries

14:05 – 14:30 **Invited**
Yuta Yoshimoto (Fujitsu, Japan)
Construction of a Robust Neural Network Potential for Large Scale Molecular Dynamics Simulations of Polymer Electrolyte Membranes

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Kei Kubota (National Institute for Materials Science, Japan)
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14:55 – 15:10 **General**
Milica Zdravkovic (Forschungszentrum Jülich GmbH, Germany)
Factors affecting phase stability in layered oxide materials

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Biwei Xiao (China Automotive Battery Research Institute Co., Ltd, Beijing, P.R. China)
Advancing High-Energy Density Layered Materials for Sodium-ion Batteries: from Basic Principles to Industrialization

15:55 – 16:10 **General**
Sourav Baiju (Forschungszentrum Jülich GmbH, Germany)
A Semi-empirical Descriptor for Open Circuit Voltage

16:10 – 16:25 **General**
Suhwan Kim (Yonsei University, South Korea)
Digital Twin-guided Design of Air Electrode Structures for Enhanced Metal-air Battery Performance

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Closing Ceremony

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18:00 – 20:00
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Poster presentation

Main Hall

Chaired by Prof. Seung-Taek Myung and Prof. Dr. Payam Kaghazchi

Monday 29 September 10:00 - Thursday 2 October 16:00

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Tai-Feng Hung (Ming Chi University of Technology, Taiwan)
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25-002
Jaesub Kwon (Pohang university of science and technology, South Korea)
Influence of Oxygen Vacancies on Defect Dynamics, Structural Integrity, and Electrochemical Performance in Layered NCM Cathode Materials

25-003
Jihee Yoon (Korea Institute of Materials Science, South Korea)
Fluorine-Free Epoxy Binder Design for High-Energy-Density Lithium-Ion Battery

25-004
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Dry-Processed Thick Electrodes for Aqueous Zinc–Iodine Batteries with Enhanced Energy Density

25-005
Jaehyuk Yang (Korea Electrotechnology Research Institute, South Korea)
Residual NMP-Induced Degradation in Sodium-ion Batteries: Benefits of Dry Electrode Processing

25-006
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Dual-salt concentration control in an in-situ polymerized gel polymer electrolyte for high-performance lithium-ion batteries

25-007
Changho Lee (Korea Electrotechnology Research Institute, South Korea)
Designing current collector interfaces for high-performance dry-processed cathodes

25-008
Taekyoung Koo (Kunsan National University, South Korea)
Optimization of Dry-Processed NCM Cathodes in Lithium Rechargeable Batteries: Effect of Binder Type on Electrochemical Performance

25-009
Minkee Kim (Kunsan National University, South Korea)
Extraction of Mn by precipitation from black mass in waste lithium battery recycling process

25-010
Joongpyo Shim (Kunsan National University, South Korea)

Preparation of C-coated Si powders from Si kerf and biomass using microwave heating for lithium ion batteries

25-011
Eunki Kim (Korea Research Institute of Chemical Technology, South Korea)
Surface Modification of OLO Cathodes via Dry-Coated Nano-LFP for Thermal and Structural Reinforcement

25-012
Dongyoon Kang (Yonsei University, South Korea)
$AgNO_3$-Preplanted Li Metal Powder Electrode: Preliminary Formation of Lithiophilic Ag and a Li_3N-rich Solid Electrolyte Interphase

25-013
Jaehyun Park (Korea Electrotechnology Research Institute, South Korea)
Performance Enhancement of Lithium–Sulfur Batteries via Polysulfide Adsorption Using a Fe_2P@MWCNT Interlayer

25-014
Seong A Park (Korea Research Institute of Chemical Technology, South Korea)
Poled $BaTiO_3$/Lithiated-SPEEK coated separator for improved safety and electrochemical performance in lithium metal batteries

25-015
Yu Jin Jo (Korea Electrotechnology Research Institute, South Korea)
Understanding the Role of Electrolyte in Lithium–Sulfur Batteries

25-016
Junghwan Sung (Korea Electrotechnology Research Institute, South Korea)
Catalytic Interface Design with MoS_2 for High-Performance Lithium-Sulfur Batteries

25-017
Hyerim Ryu (Korea Research Institute of Chemical Technology, South Korea)
Ion-Conductive LLZTO Lithium Composites for Uniform Li Deposition and Enhanced Stability in Li-Metal Batteries

25-018
You-Jin Lee (Korea Electrotechnology Research Institute, South Korea)
Controlled Nitrogen Doping in Vertically Aligned Carbon Nanotubes for Lithium–Sulfur Battery Anodes

25-019
Hawon Gu (Korea Electrotechnology Research Institute, South Korea)
Carbon-Based Triple-Structured Multifunctional Electrode Design for Polysulfide Trapping in Lithium-Sulfur Batteries

25-020
Jinhyeok Heo (Korea Electrotechnology Research Institute, South Korea)
Application of SnS_2-Based Catalytic Hosts for Enhanced Lithium–Sulfur Batteries

25-021
Ramkumar Balasubramaniam (University of Ulsan, South Korea)

A comprehensive study of the role of Metal halide in Na3SbS4 solid electrolyte for Sodium Solid State Batteries

25-022
Yuvaraj Subramanian (University of Ulsan, South Korea)
Engineering High Ionic Conductivity Na3PS4 Solid Electrolytes through W and O Co-Doping for Sodium Solid State Batteries

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Jae Won Lee (Gyeongsang National University, South Korea)
Single-Atom Fe Anchored on Graphitic Carbon Nitride for accelerated Redox Kinetics in Lithium-Sulfur Batteires

25-024
Hee Jun Kim (Gyeongsang National University, South Korea)
Lithium Salt-Modified PVDF Binder for Enhanced Lithium Sulfur Battery Performace

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Separator Coating Strategy for Room-Temperature Na–S Batteries Using Ether-Based Electrolytes

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Sung Ryul Choi (Sejong University, South Korea)
Suppressing Lithium Dendrite Penetration via Lithiophilic Interlayers in Garnet Solid Electrolytes

25-027
Seojeong Yoo (Sejong University, South Korea)
Fabrication of $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ Solid Electrolytes by Tape Casting for All-Solid-State Batteries

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Electrochemical Characterization of LICs with Ni-rich Cathodes and Direct Contact Pre-lithiated Anodes

Keynote 25-001

Scalable Electrode Engineering for High-Energy Li Batteries

Sang-Young Lee*

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Achieving high-energy-density batteries is critical to advancing the smart energy era. While much research has focused on design of electrode active materials and electrolytes, scalable electrode architectures that directly enhance areal capacity of resulting cells have received comparatively less attention. Here, we present a materials-to-manufacturing framework that achieves areal capacities exceeding 20 mAh cm^{-2} without sacrificing mechanical integrity and electrochemical performance. To meet growing demands for both performance and sustainability, we focus on PFAS-free binder systems and rheology-optimized slurry engineering. Strategies include amphiphilic bottlebrush polymers, cationic semi-interpenetrating polymer networks (semi-IPNs), and surface-functionalized nanocellulose. These binder-driven approaches prevent drying-induced phase segregation, improve electrode uniformity and manufacturing yield, and are compatible with roll-to-roll processing. The proposed platform extends beyond lithium-ion batteries to systems such as lithium–sulfur batteries and other chemistries where engineered interfacial mechanics and chemical affinity are vital for stable cycling under constrained cell conditions. This chemistry-agnostic and scalable strategy effectively bridges materials design with practical manufacturing, offering a pathway to next-generation batteries with high cell-level energy density and a reduced environmental footprint.

References

[1] S. Y. Lee et al., Upscaling high-areal-capacity battery electrodes *Nature Energy* 10 (2025) 295.

[2] S. Y. Lee et al., Material challenges facing dry-processable battery electrodes *ACS Energy Lett.* 9 (2024) 5688.

Keynote 25-002

Nanostructured Insertion Materials for Practical Li-ion Battery Applications

Naoaki Yabuuchi* and Yosuke Ugata

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Ni-enriched layered materials are widely used as electrode materials in Li-ion batteries for electric vehicle applications. Stoichiometric $LiNiO_2$, which utilizes the cationic Ni^{3+}/Ni^{4+} redox couple, is an ideal electrode material. However, its practical applications is hindered by gradual capacity degradation at the high voltage region, primarily due to Ni ion migration.[1] Recently, the critical role of non-stoichiometry and anti-site defects in $LiNiO_2$ has been highlighted. Through defects engineering, highly reversible pure Ni-based layered materials without metal substitution have been successfully developed.[1]

Another important challenge is the development of practical, high-energy Co-/Ni-free Mn-based positive electrode materials, which are essential for the widespread adoption of cost-effective electric vehicles. Nanostructured Mn-based electrode materials have emerged as promising candidates for this purpose.[2, 3] However, these materials are generally synthesized by high-energy milling, a process unsuitable for large-scale production. More recently, nanostructured $LiMnO_2$ with high-energy density (~800 Wh kg^{-1}) has been successfully synthesized through a conventional calcination process, indicating its potential for economical electric vehicle applications.[4]

To realize safe and high-energy Li-ion batteries, the use of solid electrolytes has become a critical strategy. Nevertheless, the inevitable volume changes of electrode materials during cycling pose challenges in maintaining a stable electrode-electrolyte interface. A recently developed nanostructured cation-disordered rocksalt oxide demonstrates a dimensionally invariable character, enabling excellent electrochemical reversibility with solid electrolytes.[5, 6]

These results highlight the importance of nanostructured lithium insertion materials for practical development of high-performance Li-ion batteries.

References

[1] I. Konuma *et al.*, and N. Yabuuchi, *Energy Storage Materials*, **66**, 103200 (2024).
[2] A. Kanno *et al.*, and N. Yabuuchi, *ACS Energy Letters*, **8**, 2753 (2023).
[3] Z. Yanjia *et al.*, and N. Yabuuchi, *Advanced Energy Materials*, **14**, 2304074 (2024).
[4] Y. Miyaoka *et al.*, and N. Yabuuchi, *ACS Central Science*, **10**, 1718 (2024).
[5] I. Konuma *et al.*, and N. Yabuuchi, *Nature Materials*, **22**, 225 (2023).
[6] M. Shinoda *et al.*, and N. Yabuuchi, *Journal of The American Chemical Society*, in-press

Invited 25-001

Third Generation Ni-rich Cathode Materials: Full-Concentration Gradient FG-NCM92 Cathode Materials via a Taylor Flow Reactor

Yola Bertilsya Hendri[1], Chun-Chen Yang[1,2*]

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Nickel-rich, cobalt-less layered oxide cathodes (Ni >90%) have emerged as promising candidates for next-generation lithium-ion batteries (LIBs) due to their high energy density and cost-effectiveness. However, their practical application is hindered by structural and surface instabilities, including irreversible phase transitions, transition metal (TM) dissolution, and microcrack formation during electrochemical cycling, leading to poor long-term cycling stability. To mitigate these challenges, we developed a full-concentration gradient architecture in $LiNi_{0.92}Co_{0.04}Mn_{0.04}O_2$ (FG-NCM92), synthesized via co-precipitation process using a scalable Taylor-flow reactor (TFR), followed by solid-state reaction method. The successful formation of the full-concentration gradient, featuring a Ni/Co-rich core and a Mn-enriched surface was confirmed through cross-sectional energy-dispersive X-ray spectroscopy (EDS) line scanning. Electrochemical analysis revealed that FG-NCM92 delivers enhanced initial capacity and superior cycling stability, retaining 84% of its capacity at 4.3 V and 63% at 45 °C after 100 cycles at 1C, substantially outperforming the non-gradient counterpart (NG-NCM92). Performance was further improved by incorporating 0.02 mol% Mg doping and a uniform Li_3PO_4 surface coating on FG-NCM92 (MP-2@FG-NCM92), which retained 90.7% capacity at 4.3 V and 80% at 45 °C after 100 cycles and maintained 76.3% at 4.3 V after 300 cycles at 1C. To uncover the mechanisms responsible for these improvements, we conducted density functional theory (DFT) calculations along with advanced experimental analyses, including in-operando X-ray diffraction (XRD), self-discharge assessment, thermal stability evaluation, focused ion beam-field emission scanning electron microscopy (FIB-FESEM), time-of-flight secondary ion mass spectrometry (TOF-SIMS), and post-mortem analysis. These investigations confirm that the synergistic effects of gradient architecture, Mg doping, and surface coating effectively enhance structural integrity, mitigate surface degradation, and improve electrochemical stability. Overall, our findings present a robust and scalable strategy for designing high-performance, cobalt-less Ni-rich cathodes, paving the way for the development of advanced lithium-ion batteries with superior energy density, thermal stability, and cycle life.

Keywords: Full-concentration gradient NCM92 (FG-NCM92), density functional theory, Mg doping, Li_3PO_4 Coating, Li-ion battery.

Invited 25-002

Development of High-Performance Cathodes for Lower-Cost Alternatives Beyond Conventional LIBs

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Renewable energies play a crucial role in addressing recent environmental challenges associated with global climate change. Currently, lithium-ion batteries (LIBs) are the primary power sources for portable electronics and are widely used in electric vehicles and for storing electricity generated by power plants and renewable energy sources. However, the limited and geographically concentrated lithium resources on Earth pose significant challenges to maintaining stable production levels and price stability. These factors are expected to drive up the production costs of LIBs in the near future. As a result, extensive research efforts have been dedicated to developing low-cost and efficient energy storage systems (ESSs) using earth-abundant materials. Our innovative approach combines synthesis, first-principles calculations, and advanced structural analysis techniques to efficiently discover high-performance cathode materials for low-cost rechargeable batteries. This approach enables precise confirmation of detailed reaction mechanisms and rapid optimization of electrochemical properties. We believe our findings will pave the way for the development of effective cathode materials, offering high energy density, high power output, and reduced production costs, thereby opening new opportunities for advancing battery technology.

Invited 25-003

Solid-State Li-Ion Diffusion in Lithium Insertion Materials Examined by the Diluted Electrode Method

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In our laboratory, the reaction kinetics of lithium insertion materials were investigated using the dilute electrode method.[1-3] In dilute current, the solid-state Li-ion diffusion coefficient can be estimated from the relationship between capacity retention and current density in rate capability tests.[1] In this study, solid-state Li-ion diffusion in various lithium insertion materials were examined using the dilute electrode method.

The electrode materials used were $LiCoO_2$ (LCO), $LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$ (NCM), $LiNi_{0.88}Co_{0.09}Al_{0.03}O_2$ (NCA), $LiFePO_4$ (LFP), $Li[Li_{1/3}Ti_{5/3}]O_4$ (LTO), $Li[Li_{0.1}Al_{0.1}Mn_{1.8}]O_4$ (LAMO), and $Li[Ni_{1/2}Mn_{3/2}]O_4$ (LiNiMO). The dilute electrodes consisted of 3 wt% of an active material, 85 wt% of Al_2O_3, 6 wt% of AB, and 6 wt% of PVdF.

Figure 1 shows the results of the discharge rate capability for the dilute electrodes with an active material content of 3 wt%. Intrinsic rate capability determined from the solid-state Li-ion diffusion in the active materials are quite different depending on the materials. However, no significant correlation was observed between the rate capability and their crystal structures, such as layered, spinel, and olivine structures.

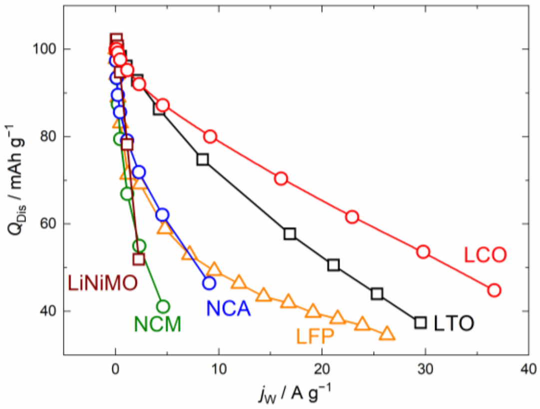

Fig. 1 Discharge capacity retention of various electrode materials examined by the diluted electrode method. Numbers in the figure indicates the active material content in the diluted electrodes.

Since the rate capability evaluated by the diluted electrodes depends significantly on the particle size, it is important to note that the particles must have the same shape and size to compare the solid-state Li-ion diffusion.[2] Based on the results of rate capability tests, we will discuss the relationship between the physicochemical properties of lithium insertion materials and the solid-state Li-ion diffusion coefficient.

References

[1] K. Ariyoshi et al., *Electrochemistry*, **89**, 157–161 (2021).

[2] K. Ariyoshi et al., *J. Power Sources*, **509**, 230349 (2021).

[3] K. Ariyoshi et al., *Electrochim. Acta*, **487**, 144192 (2024).

Invited 25-004

Overlooked Reductive Decomposition Behavior of Ionic Liquid

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Sulfonylamide-based ionic liquids have emerged as promising candidates for electrolytes in rechargeable battery systems, such as Li-ion, Li-metal, and Na-ion batteries, due to their favorable physicochemical and electrochemical characteristics.[1–3]Since the emergence of highly concentrated electrolytes as a focal point of research in electrolytes, ionic liquids containing high lithium salt concentrations have more recently been recognized for their improved electrochemical characteristics. These include an expanded electrochemical stability window, the formation of a stable solid electrolyte interphase, and significantly enhanced lithium-ion transport properties.[4,5] Despite these advances, a major hurdle remains: the excessive and unpredictable irreversible capacity losses observed in negative electrodes. This issue stems from the decomposition of "unprotected organic cations" within the ionic liquid, which contributes to poor initial Coulombic efficiency, particularly in graphite electrodes.[6]

In this presentation, we will explore in depth the physicochemical behavior and computational modeling based on $Li_x[C_2C_1im]_{1-x}[FSA]$ ($[FSA]^-$ = bis(fluorosulfonyl)amide and $[C_2C_1im]^+$ = 1-ethyl-3-methylimidazolium) ionic liquid. Our focus will be on understanding the weakening of ionic interactions between these organic cations and $[FSA]^-$ anions. We will also examine the role of anions with higher donor numbers, such as trifluoromethanesulfonate ($[OTf]^-$), and structural modifications of the organic cation, both of which have been proposed to enhance the coordination among cations, anions, and Li^+ ions.

References

[1] M. Watanabe, M.L. Thomas, S. Zhang, K. Ueno, T. Yasuda, K. Dokko, *Chem. Rev.*, 117 (2017) 7190-7239.
[2] K. Ueno, H. Tokuda, M. Watanabe, *Phys. Chem. Chem. Phys.*, 12 (2010) 1649-1658.
[3] K. Matsumoto, J. Hwang, S. Kaushik, C.-Y. Chen, R. Hagiwara, *Energy Environ. Sci.* 12 (2019) 3247.
[4] M.J. Marczewski, B. Stanje, I. Hanzu, M. Wilkening, P. Johansson, *Phys. Chem. Chem. Phys.*, 16 (2014) 12341-12349.
[5] X. Gao, F. Wu, A. Mariani, S. Passerini, *ChemSusChem*, 12 (2019) 4185-4193.
[6] S. Zhang, S. Wu, J. Hwang, K. Matsumoto, R. Hagiwara, *J. Am. Chem. Soc.* 146 (2024) 8352-8361.

Invited 25-005

Maximizing the doping effect of Al in the resynthesis of NCM cathode active material for Li-ion battery recycling

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Aluminum is either a major impurity in Li-ion battery (LIB) recycling or a popular dopant for enhancing the performance of $LiNi_xCo_yMn_{1-x-y}O_2$ (NCM) cathode active materials. Therefore, Al is often introduced to NCM by a coprecipitation method for the NCM resynthesis from LIB leachate or a solid-state method for the Al doping into NCM. We synthesize Al-doped NCM (NCMA, Al content = 0.05 and 2 mol%) using the solid-state and coprecipitation methods, denoted as NCMA(0.05 or 2)_S and NCMA(0.05 or 2)_C, respectively. Alternatively, Ni-rich NCMA with 1 mol% Al content is resynthesized using two types of industrial leachate: P-NCMA from purified leachate and R-NCMA from mother leachate. First, we focus on how the incorporation of Al affects the physicochemical and electrochemical characteristics of NCM cathode active materials depending on the two representative doping methods by using commercial reagents of Ni, Co, Mn, and Al with the Al content from an impurity (0.05 mol%) to a usual doping level (2 mol%). Further, the role and impact of Al incorporation in NCM is investigated with Al-incorporated NCM originating from the industrial LIB leachate. This work underlines the importance of impurity management and Al incorporation method in the resynthesis of high-performance NCMA from spent LIBs.

General 25-001

Toward Durable Water-in-Salt Electrolyte Lithium-Ion Batteries Under Practical Conditions

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Water-in-salt electrolytes (WiSEs) have emerged as a promising platform for safe and environmentally friendly lithium-ion batteries (LIBs). However, their practical application remains limited by parasitic hydrogen evolution reaction (HER), which leads to hydrofluoric acid (HF) formation, causing rapid capacity fade and restricting performance at low current densities. In addition, most WiSE-based LIBs operate effectively only within narrow temperature ranges due to poor thermal tolerance and accelerated degradation at elevated temperatures. In this study, we report that the Wadsley–Roth phase $Zn_2Nb_{34}O_{87}$ (ZNO) anode addresses these challenges by effectively suppressing HER. Full cells employing ZNO and $Li_{1.1}Mn_{1.8}Al_{0.1}O_4$ cathodes, combined with LiTFSI-based WiSEs, demonstrated significantly improved capacity retention at both high (5 C) and low (0.2 C) current densities. Unlike conventional anodes such as $Li_4Ti_5O_{12}$, ZNO enabled stable cycling under low-rate conditions where HER typically dominates. Moreover, temperature-dependent tests revealed that ZNO-based cells exhibited extended operating windows, with 21 m LiTFSI / 7 m LiOTf electrolyte favoring sub-ambient performance and 19 m LiTFSI / 8 m LiBETI aqueous solution supporting stable operation at elevated temperatures. These results highlight ZNO as an attractive anode for practical WiSE LIBs with enhanced durability, low-rate capability, and broad thermal operability.

Keynote 25-003

The long road of new materials towards industrialization – a show-case based on Silicon

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As an electrochemical cell is a complex and multi-level system, it is a misconception to assume that battery development can follow Moore's law. In reality, material development and its integration into commercial cells is an iterative process that often requires a decade or more, from initial scientific breakthroughs to market deployment.

The specific energy of a lithium-ion battery depends on the product of its specific charge—meaning the lithium storage capacity per unit mass—and the voltage difference between the anode and cathode. Regarding the anode, lithium and lithium compounds are already among the most reductive species in the electrochemical series. However, the carbonaceous materials used in state-of-the-art lithium-ion batteries can only store up to one lithium-ion per six carbon atoms in fully crystalline graphite, resulting in a relatively low energy density of approximately 759 $\mathrm{Ah \cdot l^{-1}}$.

Using metals or semi-metals capable of storing lithium through the formation of intermetallic phases presents a very promising alternative. In particular, silicon has shown great potential, as it could theoretically provide more than three times the charge density of graphite. However, higher charge densities come with several challenges, including structural stability, instability of the solid electrolyte interphase (SEI) layer, and specific design requirements for the cell.

This presentation will use silicon as a case study to explore the challenges and lessons learned over recent years of development. Additionally, VARTA will provide insights into its current silicon-based roadmap, highlighting the obstacles encountered along the way and showcasing exciting new results that demonstrate the potential of silicon in next-generation batteries.

Invited 25-006

Grain Size Engineering of Porous Si-Alloy Anodes for Enhanced Electrochemical Stability

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Silicon (Si) is a highly promising anode material for lithium-ion batteries (LIBs) due to its exceptional theoretical capacity (3589 mAh g^{-1}) and natural abundance.[1–3] However, its large volume change (~300%) during cycling leads to mechanical fracture and unstable SEI formation, limiting practical applications [4]. Nanostructuring is a key strategy to mitigate these issues, as Si particles below ~150 nm avoid pulverization during lithiation.[5,6] Furthermore, grain size below ~60 nm helps suppress the formation of the metastable c-$Li_{3.75}Si$ phase, which is associated with parasitic reactions in carbonate-based electrolytes.[7,8] In this work, we demonstrate a scalable approach to engineer grain-controlled porous Si alloy anodes. Amorphous Si-Al-Fe alloys were synthesized by melt spinning and recrystallized at optimized temperatures to produce uniformly distributed Si nanograins (~60 nm). Subsequent acid etching introduced a porous architecture, which improved lithium-ion kinetics and accommodated volume changes (Figure 1). The resulting anode delivered a reversible capacity of 572.2 mAh g^{-1} with 85.2% retention after 100 cycles and a high Coulombic efficiency (~99.9%). Differential capacity (dQ/dV) analysis confirmed suppression of the detrimental c-$Li_{3.75}Si$ phase. This study highlights the critical role of Si grain size control in stabilizing electrochemical performance and offers a scalable route to high-performance Si-based anodes.

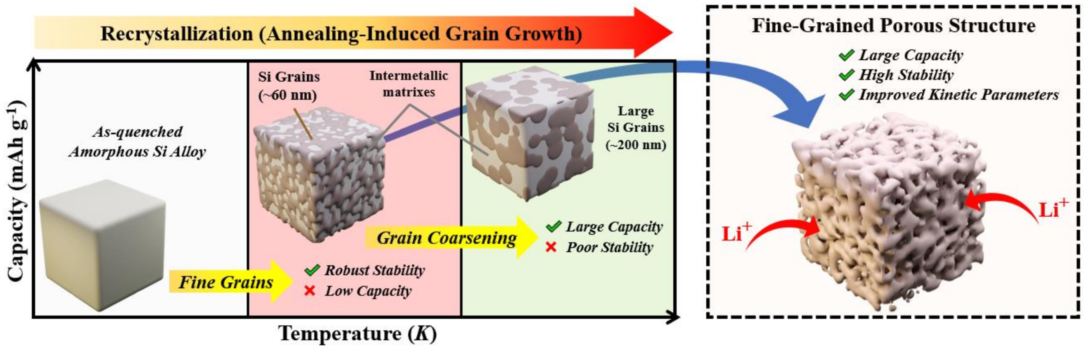

Figure 1. A schematic illustration of the fine-grained and porous Si alloys.

References

[1] J. Li, J.R. Dahn J. Electrochem Soc, 154 (2007) A156.

[2] X. Zuo, J. Zhu, P. Müller-Buschbaum, Y.J. Cheng Nano Energy 31 (2017) 113-143.

[3] G.G. Eshetu, H. Zhang, X. Judez, H. Adenusi, M. Armand, S. Passerini, E. Figgemeier Nat Commun 12 (2021) 5459.

[4] L.C. Loaiza, L. Monconduit, V. Seznec Small 16 (2020) 1905260.

[5] X.H. Liu, L. Zhong, S. Huang, S.X. Mao, T. Zhu, J.Y. Huang ACS Nano 6 (2012) 1522-1531.

[6] C. Shen, M. Ge, L. Luo, X. Fang, Y. Liu, A. Zhang, J. Rong, C. Wang, C. Zhou Sci Rep 6 (2016) 31334.
[7] H. Gao, L. Xiao, I. Plümel, G.L. Xu, Y. Ren, X. Zuo, Y. Liu, C. Schulz, H. Wiggers, K. Amine, Z. Chen Nano Lett 17 (2017) 1512-1519.
[8] P. Bärmann, B. Krueger, S. Casino, M. Winter, T. Placke, G. Wittstock ACS Appl Mater Interfaces 12 (2020) 55903-55912.

Keynote 25-004

Electrolyte Li^+ chemical potential dominates graphite anode reactions in lithium-ion batteries

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Various new electrolytes are being explored for lithium-ion batteries with higher voltage, higher rate capability, and higher safety. One of the challenges in the electrolyte development is to ensure the reversibility of graphite anode reactions. In commercial ethylene carbonate (EC) electrolyte, Li^+ is intercalated into graphite after desolvation, which has a high theoretical capacity of 372 mAh g^{-1} with excellent reversibility. On the other hand, in most of other solvents, solvated Li^+ is intercalated into graphite without desolvation. Such Li^+-solvent cointercalation leads to lower capacities and poor reversibility. Previous works show that the Li^+-solvent countercoalition can be supressed by employing (locally) concentrated electrolytes or weakly solvating electrolytes.[1] However, there has been no clear guideline on the electrolyte design that can achieve reversible Li^+ intercalation into graphite instead of Li^+-solvent cointercalation.

In this work, we report Li^+ chemical potential (m_{Li+}) in electrolytes as a quantitative descriptor of Li^+ intercalation reactions at graphite anodes. Various organic electrolytes were prepared by mixing lithium bis(fluorosulfonyl)imide (LiFSI) and organic solvents with a variety of solvation abilities. The m_{Li+} was evaluated by measuring lithium electrode potential (E_{Li}) with reference to the redox potential of ferrocene/ferrocenium (Fc/Fc^+) as an internal standard.[2] We also studied the graphite anode reactions in various LiFSI electrolytes using graphite|Li half cells. We found that graphite anode reactions varied depending on the m_{Li+} values. Li^+-solvent cointercalation generally occurred in low-m_{Li+} electrolytes, whereas reversible Li^+ intercalation occurred in high-m_{Li+} electrolytes. A threshold m_{Li+} value was identified, above which reversible Li^+ intercalation occurred without solvent cointercalation. This work provides a general guideline for designing advanced electrolytes with retaining the reversibility of graphite anode reactions.

References

[1] Y. Yamada, K. Usui, C. H. Chiang, K. Kikuchi, K. Furukawa, A. Yamada, *ACS Appl. Mater. Interfaces*, 6, 10892 (2014).
[2] S. Ko, T. Obukata, T. Shimada, N. Takenaka, M. Nakayama, A. Yamada, Y. Yamada, *Nat. Energy*, 7, 1217 (2022).

Invited 25-007

Ionic Liquid-Based High-Entropy Electrolyte for High-Reliability Lithium-Ion Batteries

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Pursuing high-energy-density and high-safety lithium-ion batteries (LIBs) necessitates the advancement of electrolytes. Currently, the widely used carbonate electrolytes face challenges in operation beyond a cell voltage of 4.3 V. Herein, an ether/ionic liquid (IL) hybrid electrolyte composed of lithium salt, *N*-propyl-*N*-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide (PMP–TFSI) IL, and dimethoxymethane (DME) is proposed to improve the safety and reversibility of 4.5-V LIBs. Unfortunately, both the IL and DME are incompatible with the graphite anode because of their unfavorable co-intercalation that cause graphite exfoliation. Accordingly, various additives are employed. The synergistic effects of combining various additives on improving the graphite performance are observed. In this electrolyte, a unique coordination structure forms, where Li^+ is surrounded by a highly complex environment consisting of DME, FEC, TTE, $TFSI^-$, $DFOB^-$, and PMP^+. The effects of this solution structure on the solid-electrolyte interphase chemistry and Li^+ desolvation kinetics are examined. The proposed electrolyte has low flammability, high thermal stability, negligible corrosivity toward an Al current collector, and the ability to withstand a high potential of up to 5 V. Importantly, this electrolyte is highly compatible with graphite and SiO_x anodes, as well as a high-nickel $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ cathode. Operando X-ray diffraction data confirm that the co-intercalation of DME and PMP^+ into the graphite lattice, a long-standing challenge, is eliminated with this electrolyte. A 4.5-V $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$//graphite full cell with the proposed high-entropy electrolyte is shown to have superior specific capacity, rate capability, and cycling stability, demonstrating the great potential of the proposed electrolyte for practical applications.

General 25-002

Ab-initio Insights into Mixed Polyanionic Cathode Materials for Sodium-Ion Batteries

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The growing demand for cheap and environmentally friendly large-scale energy storage has positioned sodium-ion batteries (NIBs) as a practical alternative to lithium-ion technologies. In particular, better cathode materials have potential to improve the performance of sodium-based batteries. Polyanionic compounds, particularly those based on phosphates, offer structural stability, safety, high ionic conductivity and in particular high voltage which makes them strong candidates for next-generation NIBs.

In this research, we utilize electrostatic analysis and first-principles density functional theory (DFT) calculations to study attractive candidates and design high-voltage mixed-phosphate cathodes namely $Na_4MM'(PO_4)_2(P_2O_7)$, where M, M' represents transition metals. Our primary focus is on Mn-based mixed-phosphate systems namely, NMnPP and their derivatives, exploring how transition-metal substitutions affect structural stability and electrochemical characteristics. The pristine NMnPP displays a theoretical voltage of approximately 3.7 V relative to Na^+/Na, which aligns with experimental observations, yet it experiences structural distortions caused by the Jahn-Teller effect from Mn^{3+} during cycling. To address these distortions, Fe substitution was implemented, resulting in N(Mn-Fe)PP. Our computational results indicate that incorporating Fe reduces the Jahn-Teller distortion, improving the structural retention of the phosphate framework throughout simulated charge/discharge cycles, and preserves a predicted operating voltage.

By predicting lattice parameters change, structural stability, voltage, and redox mechanism, we identify candidates that balances all these factors. Our computational approach can accelerate the design of high-performance, cost-effective cathodes, enhancing both the efficiency and scalability of sodium-ion batteries (NIBs).

General 25-003

A Tailored Adhesive-Conductive Interlayer for Interface Stabilization of Large-Scale Lithium Metal Powder Electrodes for High-Energy-Density Batteries

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To address the limitations in thickness and width of lithium (Li) metal electrodes produced through traditional extrusion and pressing processes, a slurry-based coating method utilizing Li metal powder (LMP) has been investigated, enabling the fabrication of ultra-thin and broad-width Li electrodes by simply tuning the coating conditions. Despite these advancements, LMP electrodes face critical challenges, including delamination of the LMP composite layer from the Cu current collector (CC) due to electrolyte infiltration at the interface and degradation of interfacial connectivity during charging/discharging cycles. To mitigate these issues, an adhesive-conductive polymer (AC-polymer) interlayer composed of poly(3,4-ethylenedioxythiophene) (PEDOT) and poly(styrene sulfonate-*co*-acrylic acid) (P(SS-*co*-AA)), was introduced between the LMP composite layer and the Cu CC to improve interfacial stability. The incorporation of the AC-polymer interlayer significantly reduced the Li stripping overpotential from 89.8 mV to 35.8 mV (a 60% decrease) and enhanced cycling stability, achieving 91% capacity retention at a 4 mA cm-2 discharging rate after 150 cycles, even in a carbonate-based electrolyte. The successful fabrication of a 300 mm-wide and 20 μm-thick slurry-coated AC-LMP electrode represents a notable advancement in the development of Li metal batteries.

General 25-004

Introducing Non-Soluble Additives in Carbonate-based Electrolytes for Lithium-Metal Batteries

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Lithium-metal batteries (LMBs) are among the most promising next-generation energy storage systems.[1] Generally, Li metal offers a high theoretical capacity of 3860 mAh g^{-1} and a very low reduction potential of -3.040 V vs. the standard hydrogen electrode (SHE), rendering it an excellent anode material candidate for achieving advanced energy densities beyond 400 Wh kg^{-1}.[2] Nonetheless, the continuous degradation of commonly used liquid electrolytes at the interface with Li metal leads to a low Coulombic efficiency (CE), dendritic growth of Li, and the formation of dead Li, which can lead to the risk of internal short-circuiting and limits the eventual cycle life, thus, imposing obstacles on their practical application.[3]

Several strategies have been proposed to improve the Li plating and stripping stability, including tailored electrolyte composition to design the solid electrolyte interphase (SEI) layer and the application of an artificial SEI layer.[4] Among these, the addition of $LiNO_3$ significantly suppresses the issues mentioned previously by the preferential reduction at the interface to form a stable inorganic SEI layer.[5] However, the poor solubility of $LiNO_3$ in conventional carbonate-based electrolytes has hindered its implementation in such systems.[6]

Herein, we report a new approach for the introduction of $LiNO_3$ in carbonate-based electrolytes for LMBs, yielding an enhanced interfacial stability and substantially increased cycle life.

References

[1] X. He, D. Bresser et al., Nat. Rev. Mater. 2021, 6, 1036-1052.
[2] T. Placke, R. Kloepsch, S. Dühnen, M. Winter, J. Solid State Electrochem. 2017, 21, 1939-1964.
[3] B. Horstmann et al., Energy Environ. Sci. 2021, 14, 5289-5314.
[4] a) Z. Tong, B. Bazri, S.-F. Hu, R.-S. Liu, J. Mater. Chem. A 2021, 9, 7396-7406; b) N. Von Aspern, G. V. Röschenthaler, M. Winter, I. Cekic-Laskovic, Angew. Chem. Int. Ed. 2019, 58, 15978-16000.
[5] Y. Liu et al., Nat. Commun. 2018, 9, 3656.
[6] H. Shin et al., Adv. Energy Mater. 2020, 10, 2001456.

General 25-005

Atomistic Configurational Optimizations in Battery Materials: Applications of the GOAC Code

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Novel battery materials such as layered oxide cathodes consist of several dopant elements that share the same crystal site. This gives raise to a vast configurational space that becomes even larger when also charging of the materials is included which gives rise to numerous alkali-metal orderings in the structure alongside the configurations of transition metal orderings. For computational studies it is pivotal to study configurations that are reasonably low in energy as otherwise incorrect material properties will be predicted. Consequently, configurational optimization software is required and we recently introduced the GOAC (Global Optimization of Atomistic Configurations by Coulomb)[1] code for that purpose. Its optimizers such as Monte Carlo and Genetic Algorithms allow GOAC to determine low energy configurations in huge configurational spaces by electrostatic energies (cf. Figure 1 a). The lowest energy configurations can be used in further DFT studies or might be analysed directly to learn about several material properties such as: alkali-metal ordering and its coupling to transition metal ordering, phase-separations during cycling (cf. single-phase to two-phase charging characteristics of $LiFePO_4$ (LFP)), and determination of the most stable crystal phase. All of these properties are essential in battery materials as they can influence the potential profile (voltage) and cycling stability. In this talk, we will show how configurational optimization by the GOAC code can be used to study battery materials. As a highlight, we will show that GOAC can correctly predict the particle size dependence of the charging mechanism of LFP[2] (cf. Figure 1 b) and that GOAC can be used to predict the most stable stacking sequence in layered oxide sodium-ion cathode materials with an accuracy of 80% compared to experimental data (Figure 1 c).

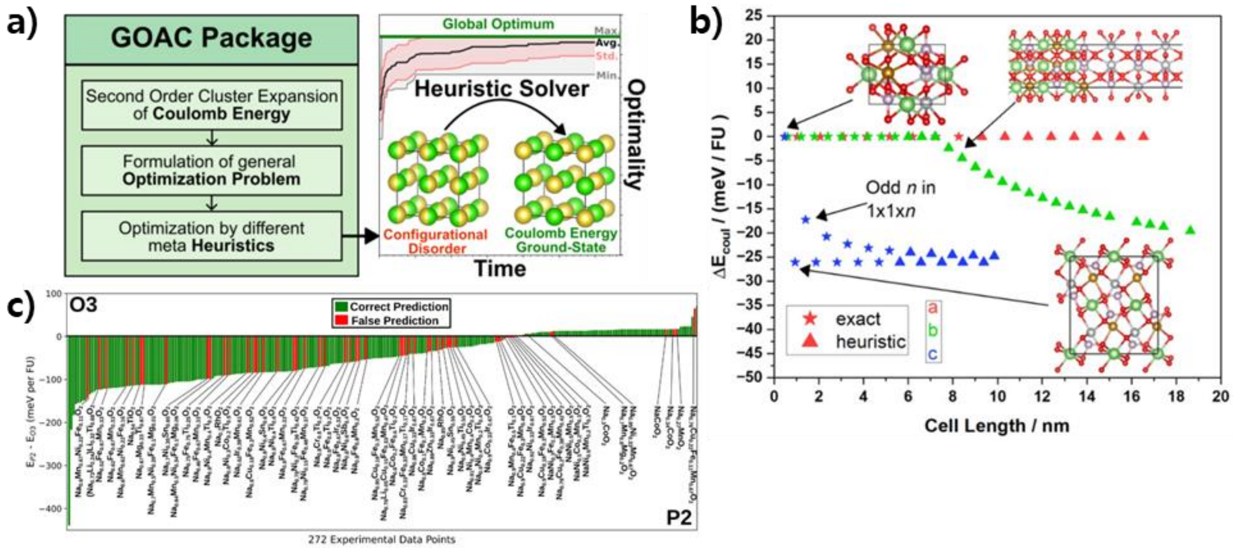

Figure 1: a) Schematic workflow of the GOAC code, b) Electrostatic prediction of two-phase charging characteristics of LFP as a function of particle size, c) Comparison of electrostatic prediction of layered oxide phase stabilities to experiment.

[1] Köster, K., Binninger, T. & Kaghazchi, P. Optimization of Coulomb energies in gigantic configurational spaces of multi-element ionic crystals. *npj Comput. Mater.* **11**, 202 (2025).

[2] Binninger, T., Ting, Y.-Y., Köster, K., Bruch, N., Kaghazchi, P., Kowalski, P. M. & Eikerling, M. H. Simulating charging characteristics of lithium iron phosphate by electro-ionic optimization on a quantum annealer. Under review in *Phys. Rev. B* (https://doi.org/10.48550/arXiv.2503.10581).

General 25-006

Adhesion and Surface Engineering of CNT Cathodes by Microwave Treatment for Enhanced Lithium–Sulfur Battery Stability

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Lithium–sulfur (Li–S) batteries offer high theoretical energy density, but their practical performance is often limited by polysulfide shuttling and electrode instability. In this work, free-standing multiwalled carbon nanotubes (MWCNTs) were used directly as cathode frameworks. To improve their structural and electrochemical properties, a short microwave-assisted post-treatment was applied prior to sulfur loading. This treatment helped reinforce the adhesion between the CNTs and the underlying Al buffer layer, contributing to improved mechanical stability. It also introduced surface functional groups that enhanced sulfur retention and limited polysulfide diffusion. SEM and TEM analyses confirmed the uniform sulfur distribution within the CNT network. Electrochemical testing showed that the treated electrodes retained over 75% of their initial capacity after 100 cycles at 0.1 C, indicating better cycling performance compared to untreated CNTs. This work contributes to the advancement of high-performance cathode materials and provides a scalable approach for developing next-generation lithium-sulfur energy storage systems.

General 25-007

Design of cathode materials using machine learning and atomistic approaches

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P2-type layered oxides are cutting-edge materials for use as a cathode in sodium-ion batteries (SIBs) due to their fast Na-ion diffusion, practical high energy density, and cost-effectiveness in production. A key weakness of applying these materials is the detrimental phase transitions toward an O-based phase, which results in capacity fading during operation. For a strategic and systematic material design, it is imperative to identify compounds that exhibit no phase transition during Na-ion extraction. Unveiling the relationship between chemical composition and structural stability is pivotal for improving the electrochemical performance of SIBs. This is an exceptionally challenging task that requires combining experimental data with theoretical approaches.

Phase transition phenomena in layered oxide materials are investigated by integrating machine learning algorithms with atomistic simulation methods. In the first stage, we constructed a comprehensive database capturing structural evolution during desodiation of around 100 P2-type layered oxide materials. Subsequently, we utilized machine learning (ML) based approaches to analyze collected experimental data. Shuffling-based feature importance analysis indicates that the initial and final transition metal (TM) ionic potentials, and initial Na concentration exhibit the largest influence on the prediction of a phase transition. A comprehensive analysis of the model demonstrates that high TM ionic potential and elevated initial Na concentration have a promotive effect on phase transition. To further investigate the intrinsic meaning of the derived features, we perform electrostatic/density functional theory (DFT) analysis on the most prominent example compounds. Combined ML and electrostatic/DFT approach provide useful insights on phase and structural stability of the P2-type layered oxides.

Keynote 25-005

Electrolyte Design of Sodium Metal Batteries

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Sodium secondary batteries have emerged as expedient lithium-ion battery alternatives due to the low costs and high abundance of sodium resources. Ionic liquids with low vapor pressure and low flammability are fascinating electrolytes for sodium secondary batteries owing to their intrinsic high safety and thermal stability.[1] In this presentation, multifunctionalities of ionic liquid electrolytes for sodium metal batteries will be comprehensively presented.

Sodium metal deposition/dissolution efficiency is improved in ionic liquids, especially at elevated temperatures. Optical microscopy reveals smooth and flat deposition of Na metal at 90 °C. Fluorination of Al substrate along with the control of crystal orientation improves the Na metal deposition/dissolution efficiency.[2] Introduction of β-alumina electrolyte further brings out the benefit of ionic liquid electrolytes. A new type of Na-S battery stably works over 1000 cycles with the dual electrolyte of β-alumina and ionic liquid.[3] Heterosite $FePO_4$ prepared by chemical desodiation of $LiFePO_4$ by O_2 serves as a positive electrode in charged-state sodium metal batteries, especially with ionic liquid electrolytes.[4]

Keywords: Sodium battery; Metal battery; Ionic liquid.

References

1. K. Matsumoto, J. Hwang, S. Kaushik, C.-Y. Chen, R. Hagiwara, *Energy Environ. Sci.*, **2024**, *12*, 3247.

2. S. Wu, J. Hwang, K. Matsumoto, R. Hagiwara, *Adv. Energy Mater.*, **2023**, *13*, 2302468.

3. D. Wang, J. Hwang, C.Y. Chen, K. Kubota, K. Matsumoto, R. Hagiwara, *Adv. Funct. Mater.*, **2021**, *31*, 2105524.

4. F. Nozaki, S. Zhang, M.H. Petersen, J. Hwang, J.H. Chang, J. M. García-Lastra, K. Matsumoto, *Energy Environ. Sci.*, **2025**, *18*, 1408.

Invited 25-008

Enhanced Na-ion Storage: Effect of Elemental Excess and Carbon Coating in $Na_4Fe_3(PO_4)_2(P_2O_7)$

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Sodium-ion battery cells present promising Key Performance Indicators (KPIs) in terms of energy, power, cycle life, cost, and safety—all of which strongly depend on the choice of active materials and cell design. Among cathode active materials (CAMs), three main classes are commonly studied: Prussian blue analogues, layered oxides, and polyanionic compounds.

Polyanionic compounds are particularly diverse and versatile. They are generally represented by the formula $Na_xM_y(X_ZO_{3z+1})$, where M is a redox-active transition metal, and X_ZO_{3z+1} denotes the polyanion group. The covalent character within these anion groups and the high electronegativity of their constituent elements enhance the ionic nature of the Na–O bond via the inductive effect. This contributes to higher operating voltages and improved thermal and air stability. Polyanionic frameworks also offer flexibility in design, enabling the use of a range of transition metals (e.g., Fe, Mn, V, Ni, Co) and polyanion types such as silicates, carbonates, phosphates, and sulfates—providing ample room for tuning the material's properties.

Sustainability, cost-effectiveness, and scalability are central to the appeal of $Na_4Fe_3(PO_4)_2(P_2O_7)$ (NFPP) as a cathode material. NFPP features a crystal structure where $P_2O_7^{4-}$ groups form one-dimensional Na^+ diffusion channels, while PO_4^{3-} and MO_6 octahedra define the channel cross-sections through corner- and edge-sharing. Three of the four sodium ions can reversibly diffuse through these channels, typically in an order determined by their coordination environment. This results in a theoretical capacity of 129 mAh/g and an average working voltage of ~3.0 V vs. Na^+/Na.

Solid-state synthesis of NFPP often yields side products such as maricite $NaFePO_4$ (NFP-m, electrochemically inactive) and $Na_2FeP_2O_7$ (NFPO, 97 mAh/g at 3.0 V vs. Na^+/Na). The concept of "elemental excess"—introducing additional sodium and/or phosphorus precursors—offers a strategy to direct phase formation. By adjusting these precursor ratios, the reaction pathway can be tuned to minimize the formation of undesired by-products. In this study, the effects of sodium and phosphorus excess in the solid-state synthesis of NFPP are systematically investigated and compared with stoichiometric conditions. Additionally, the talk will discuss how the choice of carbon coating precursor significantly impacts the material electrochemical performance, further emphasizing the importance of holistic material design in sodium-ion battery development.

Invited 25-009

Nano-crystalline $Fe_3V_3O_8$ Material as an Efficient Advanced Anode for Energy Storage Applications

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Sodium-ion battery (SIB) is a rapidly developing electrochemically rechargeable storage device and a direct substitute for Li-ion batteries. Therefore, identifying novel materials for sodium-ion storage applications is important. Efficient electrodes are particularly desirable for enhancing storage performance in battery applications. In this study, we fabricated a novel $Fe_3V_3O_8$ (FVO) anode material for Na/Li-ion storage using hydrothermal technology for the first time. The electrochemical results indicated that the initial sodiation capacity of the FVO anode is as high as 805 mA h g^{-1} at 100 mA g^{-1}, and a reversible sodiation capacity of 540 mA h g^{-1} is maintained over 200 cycles at 500 mA g^{-1}, which is more than 1.8 times the commercial hard carbon of ~300 mA h g^{-1}. In addition, the oxidation states of the chemical compound and the corresponding sodium reaction mechanism are predicted using X-ray absorption spectroscopy (XAS), X-ray photoelectron spectroscopy (XPS), and *in-situ*/*ex-situ* X-ray diffraction (XRD) analysis. Overall, the FVO material exhibited significantly higher electrochemical performance, demonstrating promising suitability for sodium-ion storage.

Invited 25-010

Thermal Stability Index of Sodium Layered Oxide Cathodes

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Sodium layered oxides provide the best electrode performance for sodium-ion batteries with high gravimetric/volumetric energy and power densities. However, their safety issues should be addressed for gird-scale use. In the present work, we systematically quantify the thermal stability of layered oxide cathodes using thermal stability index (TSI) and demonstrate a rational strategy to improve it.

Invited 25-011

Toward Practical Application of P-Type $Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ Cathodes in Sodium-ion Batteries

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Sodium-ion batteries (NIBs) have emerged as a promising alternative to lithium-ion batteries (LIBs) owing to the abundance and low cost of sodium, as well as its similar chemical properties to lithium, which enables NIBs to achieve competitive performances and remain compatible with existing LIB manufacturing infrastructure. For cathode materials, various layered oxides have been extensively studied, in which Na^+ ions occupy different coordination environments, such as octahedral (O) or prismatic (P) sites, depending on the stacking sequence. Among them, P-type structures offer a more open framework that facilitates Na^+ diffusion by reducing the energy barrier, thereby improving rate capability. However, their practical use has been constrained by relatively low sodium content, as P-type structures are typically stabilized at intermediate sodium compositions. Furthermore, P3-type materials, synthesized at relatively lower temperatures, suffer from poor crystallinity and fragile particle morphology, leading to structural degradation during cycling.

In this context, this study proposes a dual-strategy approach to overcome the limitations of P-type cathodes, focusing on P-type $Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ (P-NiMn) as a model material system for practical NIB applications. Two complementary directions were investigated as follows.

1) Water-soluble sacrificial salts combined with aqueous binders for water-stable P2-NiMn positive electrodes: Effects of incorporating water-soluble sacrificial salts (e.g., Na2CO3) in combination with aqueous carboxymethyl cellulose (CMC) binders.[1]

2) Design of high-performance P3-NiMn cathodes *via* novel synthetic routes: Using a spinel $NiMn_2O_4$ as a key precursor, which significantly enhanced cycling stability compared to conventional solid-state synthesized counterparts.[2]

Together, these findings provide new insights into the rational design and processing strategies of P-type cathodes for high-performance NIBs. Our work re-evaluates their practical potential, offering new avenues for performance enhancement and addressing their inherent limitations.

References

1) C. Lee, et al., S. Komaba, *ACS Appl. Energy Mater.* 8, 5867 (2025).

2) C. Lee, et al., S. Komaba, *International Conference on Sodium Batteries*, USA (2024).

Invited 25-012

Exploring Ni/Fe/Mn-Based Layered Cathodes for Next- Generation Sodium-ion Batteries

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Sodium, located directly below lithium in the periodic table, exhibits similar electrochemical properties but offers significant advantages in terms of elemental abundance and cost. As a result, sodium-ion batteries (SIBs) are emerging as a promising alternative to lithium-ion batteries for large-scale energy storage applications. However, the development of high- capacity, structurally stable cathode materials remains a key challenge in advancing SIB technology.

Ni–Fe–Mn-based layered oxide cathodes have shown favorable cycling performance, yet their practical implementation is limited by structural degradation, particularly the onset of monoclinic phase transitions at high voltages (>4.0 V), which lead to capacity fading. Additionally, elevating the average plateau voltage is critical for achieving higher energy densities necessary for real-world applications.

In this study, we explore the design and compositional tuning of Ni–Fe–Mn-based layered $NaMO_2$ cathode materials, aiming to optimize the balance between electrochemical performance, structural integrity, and material cost. By systematically varying the concentrations of Fe, Ni, and Na, we investigate their collective influence on the structural evolution and electrochemical behavior of $Nax(Ni–Fe–Mn)O_2$. This work provides new insights into compositional engineering strategies to overcome high-voltage limitations and enhance the overall performance of sodium-ion battery cathodes.

Invited 25-013

Anionic Redox Chemistry in Layered Sodium Manganese Oxide Cathodes

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Oxygen-redox-based layered cathode materials are key to high-energy-density sodium-ion batteries (SIBs). However, Mn-based P2/P3-type Na-poor layered oxides suffer from poor oxygen-redox reversibility and low conductivity. In our study, we explored Ni- and Co-doped P2-$Na_{0.75}[Li_{0.15}Ni_{0.15}Mn_{0.7}]O_2$ and P2-$Na_{0.6}[Li_{0.15}Co_{0.15}Mn_{0.7}]O_2$, comparing them to Ni- and Co-free P2-$Na_{0.67}[Li_{0.22}Mn_{0.78}]O_2$. Electrochemical performance was evaluated using galvanostatic cycling, neutron powder diffraction, XANES, XPS, ^{7}Li NMR, and DFT calculations. Results show that Ni enhances voltage, reduces hysteresis, and stabilizes cycling by limiting Li migration, while Co improves conductivity. This work highlights the role of Na–O–Li configurations in activating oxygen redox and provides insights into optimizing Mn-rich cathodes via tailored doping.

General 25-008

Machine Learning–Driven Phase Stability Prediction for Na-Ion Battery Cathodes

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Layered oxides have attracted considerable interest as cathode materials for sodium-ion batteries (SIBs). Accurate prediction of the most stable stacking sequence, such as the P2 or O3 phase, is essential for the rational design and optimization of these cathodes. In this work, we developed data-driven machine learning models to forecast phase stability in layered oxides. First, we assembled a comprehensive database of 270 layered-oxide compositions relevant to SIBs. From this dataset, we derived six independent descriptors, sodium concentration, transition-metal (TM) ionic radius, TM ionic potential, TM ionization energy, TM mixing entropy and cationic potential, and employed six algorithms (logistic regression, random forest, naive Bayes, *k*-nearest neighbors, support-vector machine and deep neural network) to predict the most stable phase. The deep neural network outperformed earlier two-dimensional classifiers based solely on cationic potential,[1] achieving an accuracy of 0.96, precision of 1.00, recall of 0.92 and an F1 score of 0.96. Permutation-importance and SHAP (Shapley additive explanations) analyses identified TM ionic potential, sodium concentration and TM mixing entropy as the dominant factors governing phase stability: lower TM ionic potential, higher sodium content and greater mixing entropy favor the O3 phase. Overall, our DNN-based classifier not only delivers high predictive accuracy but also yields actionable physical and chemical insights for the rational design of layered-oxide cathodes in SIBs.

References:

[1] Chenglong Zhao *et al.*, Rational design of layered oxide materials for sodium-ion batteries. *Science* 370, 708-711 (2020). DOI:10.1126/science.aay9972

Invited 25-014

From Electrode Breathing to Pressure Mapping: Operando Insights into Sodium Battery Materials

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Solvent co-intercalation—the simultaneous insertion of solvent molecules and metal ions into layered electrode materials—has long been considered a niche or even detrimental process, mostly known from graphite anodes. However, recent studies demonstrate that this phenomenon can be harnessed as a powerful design principle to modify electrode performance in sodium-ion batteries. In the first part of this presentation, we introduce recent results by Sun *et al.* [1], who investigated solvent co-intercalation in layered sulfide cathode materials (Na_xMS_2, M = Ti, V, Cr) using diglyme- and PC-based electrolytes. The study combines operando synchrotron X-ray diffraction, electrochemical dilatometry, solid-state NMR and mass change analysis to elucidate the mechanisms behind reversible co-intercalation, lattice expansion, and voltage modulation. A key insight is the observation of "opposite flux" during desodiation: while Na^+ ions leave the host structure, solvent molecules are taken up, leading to complex phase transformations and mechano-chemical interplay. These findings open new design pathways for tuning interlayer chemistry and electrochemical behavior in sodium-ion systems.

In the second part of the talk, we present a novel operando characterization platform developed for investigating mechano-chemical coupling in solid-state sodium–sulfur batteries [2]. The setup integrates simultaneous temperature control, internal pressure sensing, operando electrochemical impedance spectroscopy (EIS), and time-resolved X-ray imaging. This platform was applied to study cells containing three different solid electrolytes—Na_3PS_4 (NPS), $Na_{2.8}PS_{3.8}Cl_{0.2}$ (NaPSCl), and Na_3SbS_4 (NSbS)—each cycled over 50 charge–discharge cycles. This holistic approach allows us to monitor the evolution of internal stresses and interfacial degradation phenomena during extended cycling under realistic operating conditions. The combination of mechanical and electrochemical readouts with spatially resolved imaging paves the way for a deeper understanding of degradation mechanisms in solid-state battery systems and supports the development of mechanically robust sodium-based storage technologies.

[1] Y. Sun *et. al.*, *Nature Materials*, 2025

[2] J.-P. Hoffknecht *et. al.*, *in preparation*

Invited 25-015

Real-Time Insights: Synchrotron-Based XRD and Tomography for Unveiling Battery Mechanisms

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In situ or operando characterization techniques using synchrotron facilities, which can monitor the internal changes of batteries in real-time under actual working conditions, are of great significance for revealing the working principles of batteries, analyzing failure mechanisms, and evaluating performance of battery components. Among them, synchrotron-based XRD and X-ray tomography have attracted wide attention from researchers due to their advantages of high temporal resolution, non-destructive testing, and ease of operation. This presentation will focus on some specific applications of using synchrotron-based XRD and X-ray tomography in the research of rechargeable batteries, based on the research work of our group in the fields of metal-air batteries, lithium-ion batteries, lithium-sulfur batteries, and aqueous zinc-ion batteries. The combination of these two techniques is possible at several beam lines. It is expected that this presentation will arouse broader interest in these techniques among our peers and promote the in-depth development of related research.

References:
1. Polymeric Ionic Liquid-Enabled In Situ Protection of Li Anodes for High-Performance Li-O2 Batteries. ChemSusChem. 2025, 18(7), e202402102.
2. Addressing redox shuttling in Li-O2 batteries: Mechanistic insights by synchrotron X–ray tomography. Chemical Engineering Journal, 2024, 489, 151401.
3. A Multiscale, Dynamic Elucidation of Li Solubility in the Alloy and Metallic Plating Process. Adv. Mater., 2023, 35: 2306826.
4. The Growth of NaO2 in Highly Efficient Na-O2 Batteries Revealed by Synchrotron In Operando X-ray Diffraction. ACS Energy Lett., 2017, 2: 2440–2444.
5. Towards an Understanding of Li2O2 Evolution in Li-O2 Batteries: An In-operando Synchrotron X-ray Diffraction Study. ChemsusChem, 2017, 10: 1-9.
6. Pt/α-MnO2 nanotube: a highly active electrocatalyst for Li-O2 battery. Nano Energy, 2014, 10: 19-27.

Invited 25-016

Nuclear Magnetic Resonance in Battery Research

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This presentation will focus on Nuclear Magnetic Resonance (NMR) in battery research. NMR is extremely powerful in charactering local structures and ion dynamics in battery materials. An important feature of NMR is ability to directly observe Li and Na ions. The short-range, local structural information around Li and Na ions obtained from NMR, which is difficult to get from diffraction methods, provides a multifaceted understanding of battery material structures. However, batteries are composed of various components such as cathodes, anodes, electrolytes, separators, and conductive additives. These materials come in diverse types and forms, inorganic/organic, liquid/solid, meaning the applicable NMR techniques and the information gained from them are extensive and varied. In this presentation, we will briefly summarize what kind of information NMR can provide in the analysis of each component of battery samples with actual analysis examples, and in particular, we will report the structural analysis results of ^{7}Li and ^{23}Na solid-state NMR for the cathode materials.

Conventionally, NMR measurements of cathode materials have been difficult because of the broadening of the spectrum caused by paramagnetic interaction with unpaired electrons of transition metals. However, thanks to recent advancements in hardware, ultra-fast magic angle spinning (MAS) at speeds up to 100 kHz, and the development of the NMR pulse sequences, pj-MATPASS,[1] we can now obtain high-resolution ^{7}Li and ^{23}Na spectra.[2][3][4][5][6][7]

Here, we show an NMR analytical result of oxygen-redox-based-layered cathode materials for sodium ion batteries. Samples investigated are Mn-Based-layered materials (P2-type layered compounds $Na_{0.67}[Li_{0.22}Mn_{0.78}]O_2$ (LM) and $Na_{0.75}[Li_{0.15}Ni_{0.15}Mn_{0.7}]O_2$ (LNM). For these materials, Li ion migration associated with the extraction and insertion of Na ions are closely related to the electrochemical properties and structural stability.

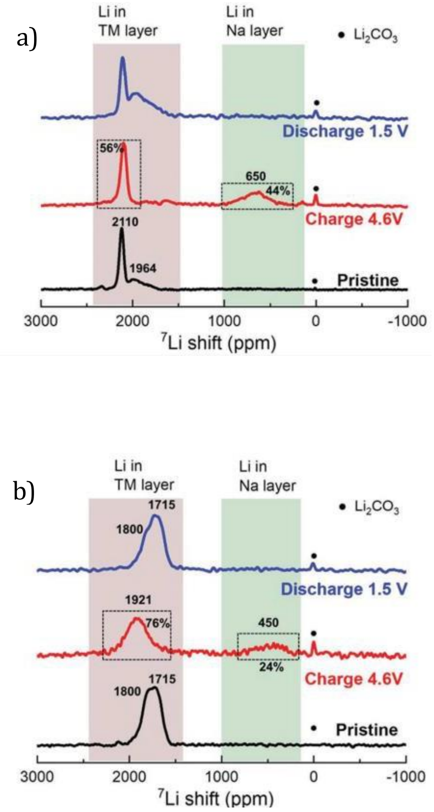

Fig. 1. ^{7}Li pj-MATPASS NMR spectra for a) LM and b) LNM.

Comparing the electrochemical performance of the two electrodes, the discharge capacity of LNM was 160 mAh/g, which was smaller than that of LM (180 mAh/g), but the average operating voltage was 3.3.V, which was higher than that of LM (2.4 V). Voltage hysteresis was also suppressed, and cycle performance was 73% at 300 cycles, a significant improvement in stability compared to LM's 18%.

In the P2-$Na_{0.6}[Li_{0.2}Mn_{0.8}]O_2$ cathode, the migration of Li from the TM site to the Na site is considered to be one of the causes of capacity reduction. Fig. 1 shows ^{7}Li pj-MATPASS NMR spectra of LM and LNM in pristine, charged (4.6 V), and discharged (1.5 V) states. ^{7}Li NMR spectra reflect the local environment of Li, with Li in the Na layer (Li_{Na}) appearing from 0- 1100 ppm and Li in the TM layer (Li_{TM}) from 1100-2400 ppm. After charging, the Li_{TM} signal decreased and a Li_{Na}-derived signal appeared at 650 ppm. After further discharge, this signal disappeared and only the Li_{TM} signal appeared again. Thus, ^{7}Li NMR provided direct evidence of Li migration (TM→Na→TM layers) during charging and discharging. The same Li migration was observed in LNM, but with differences from LM. First, during charging, the Li_{TM} signal shifted from 1715 and 1800 ppm to 1900 ppm. This is due to oxidation of Ni^{2+} to Ni^{4+}. Also, the signal intensity of Li_{Na} was 44% of the total signal intensity in LM, while it decreased to 22% in LNM, indicating that there is less Li migration into the Na layer in LNM than in LM. These results suggest that Ni doping suppresses the migration of Li to the Na layer, leading to improved cycle stability. In addition to these results, examples of Na ion desorption/insertion observed in ^{23}Na NMR will be presented.

References

[1] I. Hung, L. Zhou, F. Pourpoint, C.P. Grey, Z. Gan, *J. Am. Chem. Soc.* 134 (2012) 1898– 901.

[2] K. Shimoda, K. Yazawa, T. Matsunaga, M. Murakami, K. Yamanaka, T. Ohta, E. Matsubara, Z. Ogumi, T. Abe, *Sci. Rep.* 10 (2020) 1–12.

[3] N. Voronina, M. Shin, H. Kim, N. Yaqoob, O. Guillon, S.H. Song, H. Kim, H. Lim, H. Jung, Y. Kim, H. Lee, K. Lee, K. Yazawa, K. Gotoh, P. Kaghazchi, S. Myung, *Adv. Energy Mater.* 12 (2022) 2103939.

[4] N. Voronina, J.H. Yu, H.J. Kim, N. Yaqoob, O. Guillon, H. Kim, M. Jung, H. Jung, K. Yazawa, H. Yashiro, P. Kaghazchi, S. Myung, *Adv. Funct. Mater.* 33 (2023) 2210423.

[5] H.J. Kim, N. Voronina, K. Köster, A.Y. Kim, H.G. Jung, H. Kim, K. Yazawa, H. Yashiro, P. Kaghazchi, S.T. Myung, *Energy Storage Mater.* 66 (2024) 1–12.

[6] H.J. Kim, N. Voronina, J.H. Yu, V.A. Shevchenko, O.A. Drozhzhin, K.E. Ryou, E.Y. Jeong, A.Y. Kim, H.J. Shin, H.G. Jung, K. lhm, K.S. Lee, K. Yazawa, H. Yashiro, S.M. Bak, I.A. Presniakov, E. V. Antipov, S.T. Myung, *Energy Storage Mater.* 74 (2025) 103924.

[7] N. Voronina, K. Köster, J.H. Yu, S. Kim, A.Y. Kim, H.G. Jung, K. Ihm, K. Yazawa, H. Yashiro, A. Konarov, M. Huijben, O. Guillon, P. Kaghazchi, S.T. Myung, *Adv. Energy Mater.* 2501823 (2025) 1–16.

Invited 25-017

FOSTERING BATTERY INNOVATIONS BY ADVANCED SYNCHROTRON TECHNIQUES: CHALLENGES AND OPPORTUNITIES

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Over the years, synchrotron techniques are playing an increasingly important role in the development and innovations in battery science, due to their unique ability to provide accurate information on the electronic structure of redox active elements, local and crystalline structure, and morphological information, also in operando conditions. Despite the potential innovative outcomes of synchrotron investigations, the generation of significant developments seems hindered by the resources needed to fully and quickly exploit these capabilities and the limited cooperation between academic and industrial parties.

Several challenges can be identified for the development of more performing and sustainable batteries. First of all, it has been widely demonstrated how in most of the cases it is needed a multi-modal and/or multi-scale approach, where only a combination of techniques is able to provide a comprehensive answer to the scientific question. On the other hand, massive data production due to such approaches and coupled to the operando capabilities imply challenges in the data analysis. Moreover, the variability of several reported results points out the need of developing well defined empirical strategies, including standardized data acquisition protocols and setups and automated recognition of artifacts, to correctly identify the correlations of interest and the right descriptors to evolve towards predictor approaches.

These challenges are addressed through examples, which highlights some necessary technical developments that are expected to foster battery innovation strengthening the cooperation between academics and industries to allow a faster outcome for the society.

Invited 25-018

Microstructure-resolved Digital Twin Modeling and Simulations for Calendering Process and Dry Electrodes

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Understanding and controlling the calendering process is essential for optimizing lithium-ion battery (LIB) electrodes, as it governs key structural and transport properties. In this study, we establish and experimentally validate a physics-based virtual calendering framework using high-resolution tomographic images of $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) cathodes. By digitally compressing reconstructed electrode microstructures, we accurately simulate the impact of calendering pressure on porosity, tortuosity, and binder/active material distribution. The model shows strong agreement with experimentally calendered structures and reproduces key electrochemical trends, including impedance behavior and effective conductivity, offering a predictive tool for electrode processing optimization.

To further extend this framework toward sustainable high-energy cathode design, we demonstrate a dry-processing strategy using CNT-coated single-crystalline $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (SC–NCA), achieving 99.6 wt% active content and 4.0 g cm^{-3} density without toxic solvents. Digital twin modeling confirms the dry-processed electrodes exhibit superior pore connectivity, reduced tortuosity, and enhanced electronic/ionic transport. The integration of dry-processing with virtual calendering provides a comprehensive platform for engineering next-generation LIB electrodes with high energy density, scalability, and environmental compatibility.

References

[1] J. Lim†, J. Song†, J. Park*, Y. M. Lee* et al., Small (2025) 2410485
[2] J. K. Koo†, J. Lim†, Y. M. Lee*, Y.-J. Kim* et al., Energy Storage Materials 78 (2025) 104270

Invited 25-019

Accelerating battery innovation through operando gas analysis

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The comprehensive understanding of interface formation and evolution remains one of the most important challenges for rapid battery innovation, as these interfaces play a pivotal role on both performance and safety[1]. The gas evolution signature of interfacial processes can be highly informative, and operando gas analysis techniques have become an essential tool for accelerating battery innovation[2-6]. Electrochemical mass spectrometry (EMS) can provide quantitative information of individual processes occurring in the cell, as well as their interconnectivity (e.g., cathode- anode crosstalk and anode slippage) with high sensitivity and resolution, as it can be seen in the figure[1].

Here we present online electrochemical mass spectrometry (OEMS) studies of systems with both high-nickel cathode materials and high-voltage anode materials that show the nature, onset, extent and interconnectivity of parasitic reactions leading to cell aging using very short test protocols. Our results indicate the need for better understanding these processes in order to accurately target solutions such as electrolyte formulations, coatings, etc., to accelerate materials innovation in batteries.

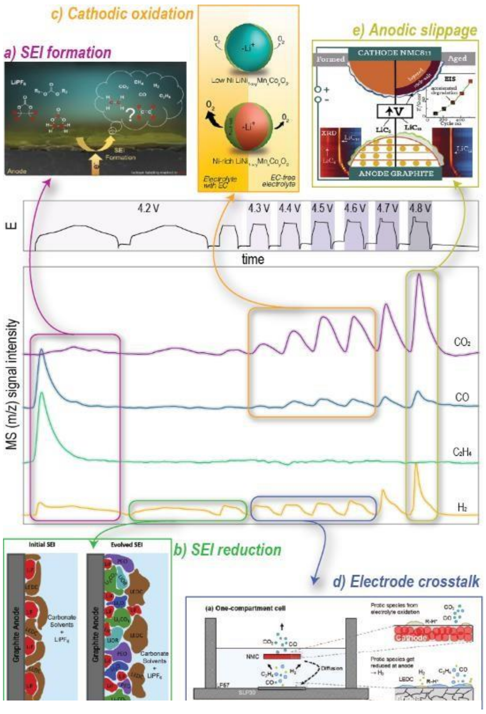

Figure 1. Operando gas analysis data (OEMS) showing voltage profile (top) alongside typical gas evolution profiles (bottom; m/z = 2 for H2; m/z = 27 for C2H4; m/z = 28 for CO; m/z = 44 for CO2) of electrochemical processes contributing to the formation/evolution of interfaces in lithium-ion batteries.

REFERENCES

[1] Temprano, I., et al., *Advanced methods for characterizing battery interfaces: Towards a comprehensive understanding of interfacial evolution in modern batteries.* Energy Storage Materials, 2024. **73**: p. 103794.

[2] Rinkel, B.L.D., et al., *Electrolyte Oxidation Pathways in Lithium-Ion Batteries.* Journal of the American Chemical Society, 2020. **142**(35): p. 15058-15074.

[3] Dose, W.M., et al., *Electrolyte Reactivity at the Charged Ni-Rich Cathode Interface and Degradation in Li- Ion Batteries.* ACS Applied Materials & Interfaces, 2022. **14**(11): p. 13206-13222.

[4] Dose, W.M., et al., *Onset Potential for Electrolyte Oxidation and Ni-Rich Cathode*

Degradation in Lithium- Ion Batteries. ACS Energy Letters, 2022. **7**(10): p. 3524-3530.

[5] Páez Fajardo, G.J., et al., *Synergistic Degradation Mechanism in Single Crystal Ni-Rich NMC//Graphite Cells.* ACS Energy Letters, 2023: p. 5025-5031.

[6] Wang, R., et al., *Influence of Carbonate Electrolyte Solvents on Voltage and Capacity Degradation in Li- Rich Cathodes for Li-ion Batteries.* Advanced Energy Materials, 2024. **14**(32): p. 2401097.

Keynote 25-006

Development of a Zn/$LiFePO_4$ Aqueous Battery System with $ZnCl_2$/LiCl Binary Electrolyte for Commercial Applications

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The global shift toward sustainable energy systems has intensified the demand for advanced energy storage technologies that offer a balance of safety, affordability, and environmental sustainability. While lithium-ion batteries are widely adopted, their reliance on flammable organic electrolytes and resource-intensive materials presents significant safety and ecological challenges. Lead-acid batteries, although cost-effective, are limited by low energy density and environmental risks associated with toxic lead content. In response, aqueous rechargeable batteries have gained considerable interest as promising alternatives. With water-based electrolytes, they enhance operational safety, reduce costs, and support green chemistry principles, while delivering competitive electrochemical performance [1, 2]. Among these, Zn/$LiFePO_4$ rechargeable aqueous hybrid-ion batteries (ReHABs) have emerged as particularly attractive. These systems integrate the benefits of zinc (Zn) and lithium iron phosphate ($LiFePO_4$) within a hybrid-ion architecture that employs both Zn^{2+} and Li^+ as charge carriers in an aqueous framework.

This dual-ion approach enables higher energy density, improved cycling stability, and enhanced safety compared to conventional aqueous batteries. The use of aqueous electrolyte eliminates flammability concerns, simplifies manufacturing, and aligns with principles of environmental sustainability, making ReHABs a strong candidate for large-scale storage.

However, several technical challenges must be addressed to unlock their full commercial potential, which require innovative solutions in electrode engineering, electrolyte optimization, and system-level design. The details of this research will be presented at the Forum.

Acknowledgements

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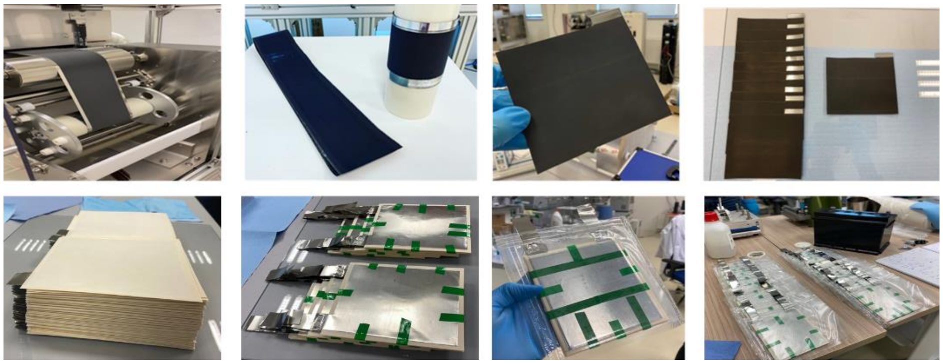

References

[1] J. Liu, C. Xu, Z. Chen, S. Ni, and Z. X. Shen, “Progress in aqueous rechargeable batteries,” *Green Energy Environ.*, vol. 3, no. 1, pp. 20–41, 2018, doi: 10.1016/j.gee.2017.10.001.

[2] X. Zeng, J. Hao, Z. Wang, J. Mao, and Z. Guo, “Recent progress and perspectives on aqueous Zn-based rechargeable batteries with mild aqueous electrolytes,” *Energy Storage Mater.*, vol. 20, pp. 410–437, 2019, doi: 10.1016/j.ensm.2019.04.022.

[3] Y. Liang and Y. Yao, “Designing modern aqueous batteries,” *Nat. Rev. Mater.*, vol. 8, pp. 109–122, 2023, doi: 10.1038/s41578-022-00511-3.

[4] N. Yesbolati, N. Umirov, A. Koishybay, M. Omarova, I. Kurmanbayeva, Y. Zhang, Y. Zhao, and Z. Bakenov, “High performance Zn/$LiFePO_4$ aqueous rechargeable battery for large scale applications,” *Electrochim. Acta*, vol. 152, pp. 505–511, 2015, doi: 10.1016/j.electacta.2014.11.168.

[5] J. Zhao, Y. Li, X. Peng, S. Dong, J. Ma, G. Cui, and L. Chen, “A Zn/$LiFePO_4$ hybrid aqueous battery,” *Electrochem. Commun.*, vol. 69, pp. 6–10, 2016, doi: 10.1016/j.elecom.2016.05.014.

[6] S. Chen, M. Zhang, P. Zou, B. Sun, and S. Tao, “Historical development and novel concepts on electrolytes for aqueous rechargeable batteries,” *Energy Environ. Sci.*, vol. 15, pp. 1805–1839, 2022, doi: 10.1039/D2EE00004K.

[7] W. Deng, G. Li, and X. Wang, “Zinc-ion battery chemistries enabled by regulating electrolyte solvation structure,” *Adv. Funct. Mater.*, vol. 34, no. 24, p. 2405012, 2024, doi: 10.1002/adfm.202405012.

Invited 25-020

Material-Level Engineering of Sustainable Organic Electrode Materials for Ultrahigh-Performance Energy Storage Systems

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The crisis on global warming, environmental pollution, and extreme climate change demands a net-zero transition, which aims to minimize the use of toxic and high carbon-emission technologies. Electrochemical energy storage is one of the largest potential applications in our modern society and will require abundant, low-cost, ultra-stable electrodes. As opposed to current Li-ion battery technologies, which rely on toxic and non-renewable metals, requiring intensive mining/processing and high-carbon-footprint manufacturing processes with end-of-life disposal issues, sustainable organic energy storage systems are top candidates. Organic electrode materials comprise only highly abundant elements, such as C, H, O, N, and S, which can meet all the criteria for next-generation batteries. They offer low cost, superior safety, environmental benignity, low-carbon-footprint production, resource abundance, and material sustainability. Most importantly, redox activity and chemical/structural features may be fine-tuned toward high energy/power density. However, to compete with inorganic-based electrodes, crucial aspects such as electronic conductivity and cycling stability still need to be improved. In this presentation, comprehensive strategies on materials design which promotes high-performance energy storage systems will be covered. Examples include manipulating organic redox-active functional groups, increasing surface areas, designing conductive structures, extending conjugated structures, and enhancing intermolecular interactions. These strategies will be highlighted together with density functional theory studies, providing proof-of-concept for the development of organic compounds as alternative electrode materials for sustainable energy storage systems, with exceptionally high energy density, rate capability, and cycling stability.

Invited 25-021

Designing Advanced Cathode Materials for Aqueous Zn-Ion Batteries with High-Rate and High-Areal-Capacity

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Although rechargeable aqueous zinc-ion batteries (RAZIBs) have been considered to be competitive candidates for large-scale energy storage, the development of this technology is stalled by the underutilization of cathode materials due to sluggish reaction kinetics, resulting in low rate perforamnce and low areal capacities that cannot meet the practical requirements. In this talk, we give three examples to obtain advanced oxide-based cathode materials. First, we reveal an efficient synthetic route to convert relatively inactive α-V_2O_5 (131 mAh g^{-1} at 0.1 A g^{-1}) into highly active Na-doped $V_8O_{20}\cdot nH_2O$ (NaVO). Benefitting from faster electron/ion transport kinetics, NaVO exhibits high capacity (383 mAh g^{-1} at 0.1 A g^{-1}) and commendable rate-performance (207 mAh g^{-1} at 8 A g^{-1}). More importantly, high-areal-capacity of 3.2 mAh cm^{-2} and remarkable cycle stability over 1500 cycles can be achieved from free-standing high-mass-loading electrode (~14 mg cm^{-2}) made of NaVO and multi-walled carbon nanotubes (MWCNTs). Second, highly electronic conductive nanocomposites comprising paramontroseite VO_2 nanoplates decorated onto MWCNT/graphene nanoribbon (MWCNT/GONR) are designed and synthesized. Paramontroseite VO_2 features with suitable open structure and metallic property. The efficient ion/electron transport properties are beneficial for enhancing the rate performance. As such, the composite sample exhibits a high capacity (428 mAh g^{-1} and 4.1 mAh cm^{-2} at 1 A g^{-1}), ultrahigh rate performance (208 mAh g^{-1} at 50 A g^{-1}), and extremely long life (10000 cycles) in aqueous Zn-ion batteries (AZIBs). Third, a layered MnO_2 with preintercalated ammonium ions (NH_4-MO) is found to exhibit single-phase charge storage behavior with minimal lattice changes during the initial cycles. Moreover, NH_4-MO more effectively induces the dissolution of Mn^{2+} and deposition of Zn-Mn species, thus promoting the Mn^{4+}/Mn^{2+} redox reaction. Therefore, NH_4-MO demonstrates the best electrochemical performance among the tested samples.

Invited 25-022

Interfacial Design for Zn metal anode towards Aqueous Batteries

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Zn metal anodes face chronic challenges from dendrite growth and hydrogen evolution reactions (HER), severely limiting their practical application. Theories centering on Zn^{2+} transport behavior have dominated explanations for high-performance of Zn anode coatings while neglecting the effect of H^+. Here, we propose a polysaccharide molecular trapping strategy to stabilize Zn anodes by decoupling Zn^{2+} and H^+ transport kinetics. The moderate trapping of Zn^{2+} guides uniform deposition by suppressing lateral migration, while the strong trapping of H^+ selectively restricts its transport, shifting the HER rate-determining step to proton diffusion. Consequently, vanadium-based full cell with XG@Zn anode work steadily at high-loading cathode, thin anode and lean electrolyte with almost no capacity fade. The combined advantages of facile fabrication and exceptional electrochemical performance underscore its commercial viability. This work establishes cation differentiation trapping as a universal design principle for Zn anode engineering, providing critical insights for next-generation Zn metal batteries.

General 25-009

Zr Incorporation into Lithium Nickel Oxides: Solid Solution or Two-Phase System

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Ni-rich cathodes such as $LiNiO_2$ (LNO) offer high theoretical capacities for Li-ion batteries, but their performance degrades upon cycling due to limiting factors such as microcracking, electrolyte decomposition, cation mixing and/or oxygen loss. A common strategy to mitigate these degradation mechanisms involves the use of doping and/or coating agents to enhance structural stability and capacity retention. Cobalt, alumina, and manganese – used in NCA and NCM cathodes – are well-known examples that improve cycling performance, although they reduce the overall theoretical capacity compared to pure LNO. Therefore, ongoing research aims to identify alternative doping and coating agents that can stabilize LNO while preserving its high theoretical capacity. Zirconium is a promising candidate, with studies reporting improved capacity retention when LNO is doped with small amounts of Zr. However, incorporating Zr into the LNO lattice remains challenging, even with low doping concentrations.

This study focuses on the incorporation of Zr into LNO using electrostatic analysis and *ab- initio* density functional theory (DFT) calculation. We analysed the synthesis route using common precursor materials, which can yield either a mixture of pure LNO and Li_2ZrO_3 (LZO), or Zr-doped LNO ($Li_xNi_yZr_ZO_2$), potentially accompanied by second phases. Our DFT calculation demonstrate that both cases, namely LNO + LZO and Zr-doped LNO (+ second phase) are energetically favoured over the precursor materials. We proposed several chemical reactions pathways for Zr-concentrations ranging from 1% up to 7%. The results suggest that low amounts (1-3%) of Zr can be incorporated into LNO if a Ni-rich secondary phase is also present. For higher Zr concentrations (4%), stabilization within LNO requires an oxygen-rich environment, such as high partial oxygen pressure during synthesis. This observation holds true even for elevated synthesis temperatures (~ 750°C) as confirmed by ab-initio thermodynamic calculations. At Zr concentrations above 4%, we find phase separation into LNO and LZO rather than Zr doped LNO. This phase separation is likely detrimental, as LZO exhibits a large band gap (> 5 eV), whereas 3% Zr-doped LNO and pure LNO have significantly lower band gaps (~0.2 eV and 0.4 eV respectively). Electrostatic calculation for large particle-like atomistic structures with more than 3000 atoms further reveal that Zr-doped LNO is energetically more stable in elongated particle geometries compared to spherical ones. Additionally, Zr ions tend to stay segregate towards the particle surface. This preference could explain experimental observations of elongated primary particles in Zr-doped LNO and may correlate with improved mechanical integrity and enhanced capacity retention.

In summary, this study provides theoretical insights into the synthesis challenges and structural advantages of Zr doping into LNO cathode materials. Our results indicate that Zr concentrations between 1-4% can be successfully incorporated under appropriate conditions, such as Ni-rich secondary phases or high oxygen partial pressure. These findings support the potential of Zr as a stabilizing dopant that retains the high capacity of LNO, offering guidance for future experimental efforts to further understand and develop advanced cathode materials for Li-ion batteries.

Keynote 25-007

Sulfide-based All-solid-state Batteries

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Lithium ion/metal batteries with liquid electrolytes still have leakage and flammability related safety concerns. Since solid-state electrolytes are in the absence of leakage and flammability issues, all-solid-state lithium metal batteries (ASSLMBs) can eliminate safety concerns. However, adopting ASSLMBs with current knowledge and development is challenging or impractical. Unlike liquid electrolytes, solid electrolytes are rigid and less capable of conforming to the electrode surfaces, often leading to high interfacial resistance. Enormous challenges exist due to various irreversible phenomena and air instability in sulfide-based all-solid-state batteries (ASSBs). Our group has developed several new sulfide-based electrolytes to mitigate their irreversible interfacial phenomena and air instability issues. The recent progress of sulfide-based all solid-state batteries (ASSBs) in Sustainable Electrochemical Energy Development (SEED) Center will be presented. The scalability and performance of the developed electrolytes and corresponding ASSBs will be also reported.

1. Y Nikodimos, et al., *Moisture Robustness of Li_6PS_5Cl Argyrodite Sulfide Solid Electrolyte Improved by Nano-Level Treatment with Lewis Acid Additives*, ACS Energy Lett., 2024, 9, 1844

2. BD Dandena et al., *Roles of Cation-Doped Li-Argyrodite Electrolytes on the Efficiency of All-Solid-State-Lithium Batteries*, Energy Storage Materials, 2024, *69(103), 305.*

3. GG Serbessa, et al., *Stabilizing the interface between Li6PS5Cl argyrodite sulfide solid electrolyte and Li via in situ formed LiF-Li_3Bi lithiophobic-lithiophilic bifunctional layer*, Energy Storage Materials, 2025, 76, 104103.

Keynote 25-008

Manipulating surface properties of garnet electrolytes for high-rate and long-cycle solid-state lithium batteries

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The solid-state lithium batteries have attracted a great deal of attention, due to their potential in enhancement of energy density as well as improvement of safety. Under such context, LLZO-based garnets become one of the most promising electrolytes. However, the surfaces of garnets are usually coated by Li_2CO_3 that is formed by attack of H_2O and CO_2 in air. Such insulating and lithium-phobic coating layers cause not only the sluggish ion transport across the interface but also the contact problems with the lithium anode. In this presentation, we will address our recent progress on manipulation of such Li_2CO_3 layers, including how to hinder its formation, how to remove it by chemical process, and how to turn it constructive by conversion reactions for good fitting with the Li anodes and the polymers. The long-cycle solid state lithium batteries with the LLZO-ceramic and LLZO/polymer composite-based cells will be given to demonstrate the effectiveness of strategy presented here. The underlying mechanism will also be addressed.

Keynote 25-009

Research Trends and Cathode Engineering Strategies for High Performance All-Solid-State Lithium–Sulfur Batteries

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Lithium-sulfur batteries (LSBs), which utilize a lithium metal anode and sulfur as the cathode active material, have been considered a promising candidate for high energy density battery systems due to their high gravimetric theoretical capacities of 3860 mAh/g and 1675 mAh/g for lithium and sulfur, respectively. However, LSBs that use flammable organic liquid electrolytes have safety concerns, such as thermal runaway and fire hazards, similar to lithium-ion batteries.

All-solid-state lithium-sulfur batteries (ASSLSBs) are next-generation batteries that incorporate nonflammable inorganic solid electrolytes, mitigating the risk of ignition while maintaining the high energy density advantage of conventional LSBs. Nevertheless, several critical challenges related to sulfur cathodes remain unresolved, including large volume changes of sulfur cathode active materials during cycling, irreversible side reactions, and low sulfur content in composite cathodes.

This presentation will highlight recent research trends and various strategies to address these issues in ASSLSBs. In addition, our group's research on improving the performance of ASSLSBs by introducing multi-cathode active materials and redox mediators, and elucidating the reaction mechanism based on in-situ analysis techniques will also be presented. Further details will be discussed at the meeting.

Invited 25-023

Single-Ion Polymer Electrolytes based on Polysiloxane for Next-Generation Lithium Batteries

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Polymer electrolytes based on polyethylene oxide (PEO) are the only commercial solid-state electrolyte system so far. However, the relatively low ionic conductivity at ambient temperatures, the remaining risk of lithium dendrite formation, and the limited electrochemical stability towards oxidation have hindered a widespread use so far.

Single-ion conducting polymer electrolytes (SIPEs) with an enhanced chemical design to withstand electrochemical oxidation, containing small molecules with a high dieletric constant to (partially) decouple the charge transport and the segmental dynamics of the polymer, provide an approach to overcome these limitations – not least as the single-ion conductivity can theoretically prevent a dendritic lithium deposition.

Herein, our progress in this field will be presented, with a specific focus on polysiloxane-based SIPEs. The talk will highlight the great versatility of this electrolyte class, enabling the realization of high-performance SIPEs for lithium-metal batteries (and beyond), the potential use as simple coating layer to stabilize the electrode│electrolyte interface, and the “first-step” scale-up of the synthesis to the kg-level.

Invited 25-024

Comprehensive study of ionic mobility in hybrid solid-state electrolyte for the next generation of batteries

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All-solid-state batteries, combining a solid ionic conductor electrolyte and a metallic lithium anode, stand as a promising high energy density system among alternative technologies to Li-ion energy storage systems [1,2]. However, excellent ionic conductivity, comparable to those of state-of-the-art liquid electrolytes, is crucial to enable this technology. In the past 50 years, several ceramic materials have been reported with excellent bulk lithium ionic conductivities, up to 25 mS.cm^{-1} [3]. Their integration in devices now raises multiple challenges. One is to maintain such high conductivities in the processed form, *i.e.* as a densified ceramic layer for the separator and as a composite also containing the active material and an electronic conductor for the positive electrode. Intimately mixing an oxide based ionic conductor with a polymer or gel type conductor to decrease the resistance at grain boundaries has been proposed to achieve high ionic conductivity without compromising the integrity of the materials. This opens new possibilities for processing, at lower temperatures and pressure, including the possibility to prepare self-standing films with thicknesses approaching 50 µm [4]. However, it also raises new questions about the nature and properties of interfaces in these hybrid materials, and about the effect of the composite architecture on the ion conduction pathways. To investigate the key parameters of the assembly and their influence on the resulting electrochemical properties, we conducted an extensive study using impedance spectroscopy and electron microscopy on cubic Al-doped $Li_7La_3Zr_2O_{12}$ (LLZO) material, one of the most promising solid electrolytes. Among various parameters such as duration, temperature, pressure, morphology, proportion, solvent, and additives, we identified the optimal conditions for their syntheses and application as efficient electrolyte materials. Importantly, the transport of Li^+ ions in these composites was studied using EIS, revealing a conductivity value of 10^{-4} S/cm for cubic LLZO with PPC, DMF and $LiClO_4$ at a compaction level of 76 %. Moreover, by investigating both complex impedance and complex permittivity behaviour, over a wide range of frequencies, we demonstrated that organic/inorganic interfaces exhibit significant polarization when the dielectric constants of the two materials differ greatly. This suggests that Li^+ transport primarily occurs through the connected PPC-DMF-$LiClO_4$ network, where the interface tortuosity has a substantial impact. To fully describe this behaviour, following our previous investigations [5], a comprehensive transmission line model was used. Conversely, when interface polarization is minimal, Li^+ transport occurs through both the interface and the connected PPC-DMF-$LiClO_4$ network, resulting in better ionic percolation with reduced tortuosity.

[1] Wang, Y.; Chen, Z.; Jiang, K.; Shen, Z.; Passerini, S.; Chen, M. Accelerating the Development of LLZO in Solid-State Batteries Toward Commercialization: A Comprehensive Review. Small. John Wiley and Sons Inc, August 28, 2024. https://doi.org/10.1002/smll.202402035.

[2] Sung, J.; Heo, J.; Kim, D. H.; Jo, S.; Ha, Y. C.; Kim, D.; Ahn, S.; Park, J. W. Recent Advances in All-Solid-State Batteries for Commercialization. Materials Chemistry Frontiers. Royal Society of Chemistry, January 31, 2024, pp 1861–1887. https://doi.org/10.1039/d3qm01171b.

[3] Mizuno, F.; Hayashi, A.; Tadanaga, K.; Tatsumisago, M. High Lithium Ion Conducting Glass-Ceramics in the System Li_2S-P_2S_5. Solid State Ion, 2006, 177 (26-32 SPEC. ISS.), 2721–2725. https://doi.org/10.1016/j.ssi.2006.04.017.

[4] Ock, J. Y.; Fujishiro, M.; Ueno, K.; Kawamura, I.; Tatara, R.; Hashimoto, K.; Watanabe, M.; Dokko, K. Transport Properties of Flexible Composite Electrolytes Composed of $Li_{1.5}Al_{0.5}Ti_{1.5}(PO_4)_3$ and a Poly(Vinylidene Fluoride- Co-Hexafluoropropylene) Gel Containing a Highly Concentrated $Li[N(SO_2CF_3)_2]$/Sulfolane Electrolyte. ACS Omega, 2021, 6 (24), 16187–16193. https://doi.org/10.1021/acsomega.1c02161.

[5] Naboulsi, A.; Nguyen, G. T. M.; Franger, S.; Fichet, O.; Laberty-Robert, C. Characterization of Li^+ Transport through the Organic-Inorganic Interface by Using Electrochemical Impedance Spectroscopy. J Electrochem Soc, 2024, 171 (2), 020523. https://doi.org/10.1149/1945-7111/ad2595.

Invited 25-025

Composite Electrolytes for Solid-State Lithium Batteries

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Solid-state lithium batteries require thin-film solid electrolytes with robust and high ionic conductivity properties. Herein, this study demonstrates the superior performance of composite solid electrolytes when assembled with electrolyte-incorporated composite cathodes. High salt concentration enhances Li^+ diffusion and forming LiF-rich solid-electrolyte interphase that prevents dendrite growth. Integrating lithium-aluminum-titanium-phosphate (LATP) particles further improves Li^+ transport by modifying the [Li^+-solvent] complexes and retricting anion mobility. A solid electrolyte membrane of high mechanical strength is produced through incorporating the electrolyte precusor into a poly(tetrafluoroethylene) film and presents an ionic conductivity of 1.4×10^{-3} S cm^{-1} at 30°C. Combining the electrolyte precusor with $LiFePO_4$, $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$, or $LiFePO_4$-LATP agglomerate produces composite cathodes. Solid-state cells are assembled by inserting the electrolyte membrane between a Li-anode and a composite cathode. A resulting Li||$LiFePO_4$ cell retains 95.4% capacity after 4000 cycles of galvanostatic charge-discharge at 1 mA cm^{-2} with coulombic efficiency of ~100%.

Invited 25-026

Compatibility of polyimide separator with full cyclic carbonate electrolytes

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The electrolytes in current Li-ion batteries (LIBs) are composed of cyclic carbonate like ethylene carbonate (EC) and acyclic carbonates such as dimethyl carbonate (DMC) and diethyl carbonate (DEC). The flashing point of acyclic carbonates is around 20 ºC (17 ºC for DMC, 25 ºC for DEC), on the other hand, that of cyclic carbonates is above 400 ºC (465 ºC for EC). Thus, the acyclic carbonates play a critical role in safety concerns in LIBs.

Full cyclic carbonate electrolytes are considered to be safer than current electrolytes containing acyclic carbonates. However, the current polypropylene (PP) separator is not compatible with the full cyclic carbonate system due to low wettability (Fig. 1).

In this study, a polyimide (PI) separator is developed. The PI separator revealed high compatibility with EC:PC (propylene carbonate) electrolyte (Fig. 1), resulting in superior battery performance compared with PP separator. The PI separator would be a vital component to build a safe LIBs.

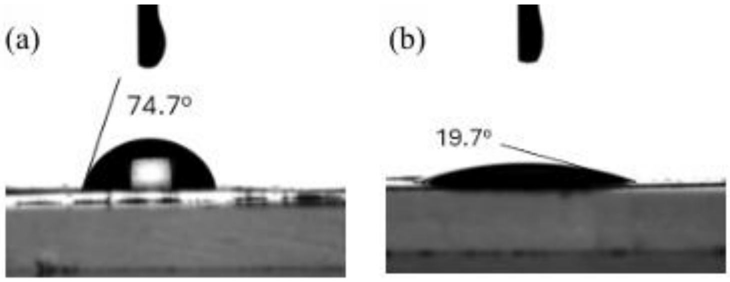

Fig. 1 Contact angle of (a) PP separator and (b) PI eparator with 1M $LiClO_4$/EC:PC electrolyte

Invited 25-027

3D Porous Single-Ion Conductive Polymer Electrolyte for High-Performance Lithium-Metal Batteries

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The growing demand for high-energy-density energy storage has brought lithium-metal batteries (LMBs) to the forefront, owing to the ultrahigh theoretical capacity of lithium metal. However, conventional liquid electrolytes used in LMBs pose critical challenges, including leakage, the formation of hazardous lithium dendrites, and limited electrochemical stability—all of which raise serious safety concerns. To address these issues, polymer electrolytes (PEs), particularly single-ion conductive polymer electrolytes (SICPs), offer a promising alternative. By selectively transporting lithium ions while immobilizing anions, SICPs help suppress concentration polarization and dendrite growth. Yet, most SICPs suffer from low ionic conductivity at room temperature, hindering their practical deployment.

In this study, we developed a three-dimensional (3D) porous SICP by sulfonating poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and integrating it with an ether-based polymer network (EPN), referred to as SICP-EPN. PVDF-HFP was selected for its electrochemical stability, mechanical flexibility, and modifiability. The sulfonated PVDF-HFP matrix enabled lithium-ion conduction, and was subsequently embedded with an EPN composed of poly(ethylene glycol) methyl ether acrylate (PEGMEA), dimethoxytetraethylene glycol (G4), succinonitrile (SN), and lithium salts. The resulting 3D architecture facilitated efficient, delocalized Li^+ transport while mitigating dendrite formation.

The optimized SICP-EPN electrolyte achieved a high ionic conductivity (~10^{-4} S cm^{-1} at 30 °C), an improved lithium-ion transference number (t_{Li+} = 0.58), and a wide electrochemical stability window (>4.9 V *vs.* Li/Li^+). Symmetric lithium cells using this electrolyte showed stable cycling with low polarization, while Li/SICP-EPN/NCM811 full cells delivered a high initial discharge capacity (189 mAh g^{-1} at 0.1 C) and retained 82% of their capacity after 250 cycles at 0.5 C. This work demonstrates the potential of combining SICP architectures with ether-based polymer networks to enhance the safety, performance, and viability of lithium-metal batteries for next-generation energy storage systems.

Invited 25-028

High-performance polymer-based solid-state electrolyte for lithium metal batteries

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Polymer solid-state electrolytes (SSEs) offer significant advantages for next-generation lithium metal batteries, including flexibility, ease of processing into thin films, and compatibility with high-voltage cathodes and lithium metal anodes. Their thin thickness (< 20 μm) minimizes inactive mass, enabling high energy densities exceeding 400 Wh kg^{-1}. However, they still face critical challenges: 1) A fundamental thickness-performance trade-off, where reducing thickness compromises mechanical strength and ionic conductivity; 2) Low room-temperature ionic conductivity (often $<10^{-4}$ S cm^{-1}) due to polymer crystallinity (e.g., PEO), necessitating elevated operating temperatures; 3) Low Li^+ transference numbers ($t_{Li+} < 0.4$), leading to concentration polarization and dendrite growth; 4) Poor interfacial stability with electrodes, causing high resistance and capacity fade, especially with high-loading cathodes or at low temperatures; 5) Mechanical fragility in ultrathin forms, risking short circuits.

To address these challenges, our group employed innovative material strategies.

Firstly, the multifunctional nanofillers are developed. For example, a record-thin (3 μm) hybrid SSE was fabricated by impregnating a substrate containing lithium sulfonate-functionalized mesoporous SiO_2 nanoparticles (SiO_2-SO_3Li) with a VEC-PEGDA copolymer/LiTFSI precursor, followed by UV curing. TheSiO_2-SO_3Li particles enhanced wettability, provided anion ($TFSI^-$) trapping sites via surface groups, and offered cation exchange channels, boosting ionic conductivity (1.77×10^{-4} S cm^{-1}) and t_{Li+} (0.65). The composite structure also provided robust mechanical properties (29 MPa strength, 95% elongation) and thermal stability (no shrinkage at 180°C). Coupled with a NCM811 cathode and lithium metal anode, the pouch cells demonstrated excellent cycling stability (88.6% retention after 100 cycles) and rate capability at room temperature.

Secondly, a ion-rectifying honeycomb-like composite skeleton embedded with multifunctional nanofillers mosaics was designed and fabricated. For example, the BNNFs provide Lewis acid sites to immobilize $TFSI^-$ anions, while LiNafion domains facilitate rapid Li^+ exchange via sulfonic groups. This synergy promotes Li^+ dissociation, achieving ultrahigh ionic conductivity (5.5×10^{-4} S cm^{-1}), high t_{Li+} (0.85). The honeycomb structure also provides exceptional mechanical strength (30 MPa tensile strength) and puncture resistance. Paired with high-loading NCM811 cathodes (12 mg cm^{-2}) and thin Li anodes (40 μm), pouch cells delivered high energy density (838 Wh L^{-1}) and stable cycling (92.2% retention after 100 cycles at 25°C), even operating at -10°C without external pressure.

In summary, these strategies transform passive reinforcement matrices into active, ion-regulating frameworks. By designing composite architectures that decouple ionic conduction from mechanical properties and enhance interfacial stability, the authors successfully broke the thickness-performance deadlock, enabling high-performance, pressure-free ultrathin polymer SSEs for practical solid-state batteries

References

[1] Kexin Liu, Hui Cheng,Zhuyi Wang*, Yin Zhao, Yingying Lv, Liyi Shi, Xuesong Cai, Zhongling Cheng, Haijiao Zhang*, Shuai Yuan*. A 3 μm-Ultrathin Hybrid Electrolyte Membrane with Integrative Architecture for All-Solid-State Lithium Metal Batteries. Advanced Energy Materials, 2024, 2303940.

[2] Kexin Liu, Yun Xie, Tao Ding, Cong Guo,Pan Guo,Jie Liu,Xing Liu, Liyi Shi, Zhihao Pan, Xuesong Cai, Jianming Wang, Zhuyi Wang,* Guosheng Shi,* Shuai Yuan*. High-Strength Ultrathin Solid-State Electrolyte with Ion-Rectifying Honeycomb-Like Skeleton for Lithium Metal Batteries Free from External Pressure. Advanced Functional Materials, 2025, e11558.

Invited 25-029

PVDF/NASICON-Based Composite Solid Electrolytes for Enhanced Sodium-Ion Battery Performance

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Sodium-ion batteries (SIBs) have gained significant attention as a promising alternative to lithium-ion batteries, owing to the natural abundance of sodium. However, the flammability and leakage risks associated with liquid electrolytes present major barriers to their widespread deployment. In this context, solid-state electrolytes offer a safer and more stable solution, with improved thermal and mechanical properties that have drawn considerable scientific interest.

In this study, we develop composite solid-state electrolytes (CSEs) comprising a PVDF-based polymer matrix combined with NASICON-type ceramic fillers and inert additives, fabricated via a simple solution-casting method. We find that the incorporation of sodium salt (NaPF6) significantly influences the porous and crystalline nature of the polymer matrix, thereby affecting the ionic conductivity of the CSE.

The resulting CSE exhibits satisfactory thermal stability and robust mechanical strength, including high tensile strength and elongation, confirming its structural integrity. Electrochemical testing of a pouch-type full cell, comprising a transition-metal-based cathode, hard carbon anode, and the CSE, demonstrates a discharge capacity of 85 mAh g^{-1} at 0.2 C, with over 90% capacity retention after 200 cycles. Additionally, the cell maintains over 70% capacity retention at 5 C/0.2 C, indicating favorable rate capability. The optimized balance of sodium salt, active, and inactive fillers in the CSE contributes to these enhanced electrochemical properties. Overall, the improved safety profile and reliable performance of the full cells underscore the strong potential of the developed CSE for future applications in SIBs.

Invited 25-030

Engineering transport properties in polymer composite electrolytes by filler particle additions

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The interactions between filler particles and the polymer–anion salt matrix in composite polymer electrolytes (CPEs) play a critical role in determining ionic conductivity in these hybrid materials. Tailoring the physical and chemical properties of the fillers—including lattice defects, surface charge, dielectric constant, and surface defect density—provides an effective strategy to engineer and optimize ion transport. This presentation will share recent results from our research, highlighting: (i) the role of lattice defects in generating macroscopic polymer transport channels; (ii) polarization effects induced by high–dielectric constant oxides; and (iii) the impact of surface–defective 2D MXene additives. These findings highlight the versatility of hybrid solid-state materials and their potential for advancing the design of high-performance all–solid-state batteries.

Invited 25-031

An Overview on Polymer-based Electrolytes with High Ionic Mobility for Safe Operation of Solid-State Batteries

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Commercial alkali metal ion secondary batteries utilise liquid electrolytes as ion transport media, which are based on toxic and volatile organic carbonate solvents. The tendency for these electrolytes to undergo side reactions, oxidative decomposition, gas production, and combustion is exacerbated at high temperatures. The most promising solution at present is to switch to all-solid-state designs that utilise polymer materials, films, ceramics, and low-volatile, environmentally friendly additives. The transformation from liquid- to solid-state architecture is expected to improve the safety, fabrication, and temperature stability of energy storage devices, particularly if the constraints of low ionic conductivity, low cation transport properties, and stringent processing conditions are overcome [1]. Here, an overview is provided of the recent developments in our laboratories on innovative polymer-based electrolytes that enable high ionic mobility, particularly attractive for safe, high-performance, solid-state alkali metal ion batteries. These electrolytes were obtained using different techniques, including solvent-free extrusion combined with UV-induced photopolymerisation. Electrochemical performances in lab-scale devices can be readily improved by using different polymer formulations, including PVDF-based ones and PEO-PC blends, and utilising various plasticisers, such as room-temperature ionic liquids (RTILs), specific low-volatile additives, and bio-sourced components [2-4]. The optimised formulation ensures good compatibility with lithium metal negative electrodes and high Ni-content NMC cathodes. The study helps identify suitable electrolyte formulations that grant good ionic conductivity, electrochemical stability windows, and elastic moduli, thus ensuring their practical application in all-solid-state Li-based batteries.

References

[1] Kim, T et al. J. Mater. Chem. A 17 (2019) 2942-2964
[2] Lingua, G et al. Macromolecules 54 (2021) 6911–6924
[3] Gastaldi, M et al Materials Today Energy (2025) 101947
[4] Gambino, F Journal of Power Sources Advances (2024) 30, 100160

Invited 25-032

An elastic solution to solid polymer-based Li metal batteries

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The flexibility of Solid Polymer Electrolytes (SPEs) can enable good manufacturability and can form good electrode-electrolyte interfaces. However, they often suffer from low ionic conductivities ($<10^{-5}$ S cm^{-1}) at temperatures lower than its melting point and poor electrochemical stabilities especially against high voltage (>4.0 V vs Li) cathode materials. In addition, polymer-in-salt systems typically have low Li^+ transference numbers (<0.4) resulting in steep ion concentration gradients and lower cyclability. The low ionic conductivity in solid-polymer systems is due in part to the inherent crystallinity; the polymer-in-salt forms either pure polymer or complex crystals which immobilises Li^+ reducing cationic movement resulting in poor ionic conductivities and transference numbers. In this work, the ionic conductivity of prototypical SPEs was investigated and a strategy of designing an all-solid amorphous SPE will be discussed. The amorphous SPE possess ionic conductivities of 10^{-4} S cm^{-1} and high transference numbers (>0.7) in all-solid-state, surpassing the performance of commercial SPE systems. The amorphous SPE has also been applied to a solid-state Li|$LiFePO_4$ cell, showing stable charge-discharge profiles over 200 cycles with an average Coulombic efficiency of 99.6 %.

Invited 25-033

Preparation and Application of Polymer Solid-State Electrolyte

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The lithium metal battery (LMB) is regarded as one of the ideal candidate materials for the next-generation high-energy-density energy storage systems, owing to the extremely high theoretical specific capacity and the lowest redox potential of the lithium metal anode (LMA).[1] However, this system faces severe challenges: the continuous interfacial side reactions between LMA and organic electrolyte lead to the irreversible loss of active Li^+, resulting in the dynamic instability of the electrode/electrolyte interface, accelerating the capacity decay, and significantly reducing the cycle life of LMBs. At the same time, the problem of dendrite growth caused by uneven Li^+ deposition also poses a serious threat to the safety of LMBs.

Aiming at the above bottlenecks, the solid-state electrolyte (SSE) shows significant advantages. Unfortunately, the point-to-point electrical contact at the interface between inorganic SSE and electrode hinders the continuity of ionic transport. Polymer electrolytes are expected to ensure continuous interfacial contact due to their excellent mechanical toughness. However, traditional polymer matrices such as PEO and PVDF have deficiencies in ionic conductivity and electrochemical stability.[2]

Poly(ionic liquid) (PIL) as an alternative material can achieve the integration of functional characteristics through the design of monomers and polymer structural regulation. Furthermore, PILs can not only inherit the characteristics of ILs such as a wide electrochemical stability window, high thermal decomposition temperature and low glass transition temperature but also the excellent mechanical processability and interfacial adaptability of the polymer matrix.[3] Herein, we propose the synthesis of functional monomers and polymer structural regulation to realize PIL-based electrolytes with both excellent electrochemical performance and physicochemical properties. We have also found that PIL can achieve obvious effects in preparing a controllable artificial interfacial layer through in-situ coating on the electrode, realizing an efficient ionic transport channel and physically blocking the continuous interfacial side reactions between the electrolyte and electrode, providing new technical routes for the development of solid-state LMBs with high safety and long cycle life.

Keywords: Lithium metal battery; Solid-state electrolyte; Poly(ionic liquid); Molecular structure design

References:

[1] Wang S H, Yin Y X, Guo Y G* et al., Advanced Materials, 2017, 29(40): 1703729.

[2] Xue Z G*, He D, Xie X L*, Journal of Materials Chemistry A, 2015, 3(38): 19218-19253.

[3] Liu L W, Xu J J*, Wu X D*, et al., ACS Applied Materials & Interfaces, 2024, 16(7): 8895-8902.

General 25-010

Polysiloxane-Based Single-Ion Conducting Polymer Electrolyte for Na-Metal Batteries

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Sodium-metal batteries (SMBs) are regarded as promising next-generation energy storage systems, but continue to face critical challenges such as an unstable solid electrolyte interphase (SEI) formation and dendritic sodium metal growth.[1,2] These issues primarily arise from the intrinsic reactivity of sodium towards classic liquid electrolyte components and the appearance of extensive charge concentration gradients upon cycling. To address the latter, the development of advanced electrolyte systems with high sodium-ion transference numbers (t_{Na+}) is crucial to address these challenges.

Herein, we present a novel polysiloxane-based single-ion conductor (NaPSiO). Blending NaPSiO with poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) and incorporating 45 wt.% organic carbonate solvents yields a freestanding membrane (NaPSiOM) with high ionic conductivity (0.35 mS cm^{-1} at 40 °C) and a wide electrochemical stability window (>4.4 V). Remarkably, symmetric Na||Na cells employing NaPSiOM demonstrate stable cycling for over 2,000 h, which is attributed to its single-ion conducting behavior and the formation of a robust interphase on the sodium surface. Moreover, Na | NaPSiOM | $Na_3V_2(PO_4)_3$ full-cells exhibit exceptional long-term cycling stability (96% capacity retention after 1,000 cycles) and outstanding rate capability up to 8C. Notably, an excellent performance is achieved even with high cathode mass loadings of up to 20 mg cm^{-2}, further highlighting the great potential of NaPSiO for next-generation SMBs.

Reference:

[1] L. Yan, G. Zhang, J. Wang, Q. Ren, L. Fan, B. Liu, Y. Wang, W. Lei, D. Ruan, Q. Zhang, Z. Shi, Energy Environ Mater 2023, 6, e12523.

[2] H. Che, S. Chen, Y. Xie, H. Wang, K. Amine, X.-Z. Liao, Z.-F. Ma, Energy Environ Sci 2017, 10, 1075.

Invited 25-034

Unsupervised Framework for Automating the Analysis of Structure and Diffusion in Solid-State Electrolytes from Atomistic Simulations

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Solid-state electrolytes (SSEs) present a promising alternative to conventional liquid organic electrolytes in lithium-ion batteries. Their non-toxic, non-flammable nature enhances safety and may boost energy density by allowing the use of metallic lithium anodes. Numerous candidate materials exhibiting high ionic conductivity (IC) have already been identified. However, optimizing their performance while maintaining chemical and mechanical stability demands a deep understanding of the mechanisms driving their fast IC. Atomistic simulation techniques, including *ab initio* molecular dynamics (AIMD) and classical molecular dynamics (CMD), have played a key role in this endeavour. When combined with structural and electrochemical spectroscopy, these methods have enabled detailed insights into ionic diffusion pathways across specific sublattices in host materials. Still, external influences like temperature, pressure, and aliovalent doping can drastically alter the positions, geometries, and connectivity of these diffusion sites. Furthermore, extremely rapid ionic transitions complicate the precise identification and categorization of diffusion sites from both experimental and computational perspectives.

A closely related challenge is understanding how collective ion motion influences IC, a process heavily dependent on accurately mapping diffusion pathways. The standard approach, which employs van Hove correlation functions, is limited to pairwise correlations [1,2]. This limited perspective fails to capture multi-ion dynamics and concentration effects that are especially relevant in SSEs with high mobile ion contents [3,4]. While cooperative diffusion can lower activation energies and potentially enhance IC [3], effectively identifying and analysing these so-called diffusion "chains" across long simulation runs with hundreds or thousands of atoms remains a difficult task.

To meet these challenges, the development of advanced computational tools that can analyse atomistic trajectories with minimal supervision has become crucial in many areas of materials science. Several schemes requiring prior knowledge of crystallographic site positions, geometries, and cutoff thresholds have been proposed for the post-processing of CMD and AIMD – derived data [5,6]. However, these methods are often sensitive to structural variations and thermal noise during the simulation run. More recently, unsupervised methods that rely on fewer predefined structural parameters have emerged [7], though they typically demand high- frequency data sampling, raising computational costs.

In this work, we present a novel, density-based unsupervised approach that enables accurate and efficient identification and classification of diffusion sites. This method provides a robust framework for analysing atomistic trajectories and captures both independent and collective behaviours of diffusing ions without requiring prior crystallographic knowledge or on-the-fly tracking of crystallographic sites geometries. By bridging the gaps in existing schemes, our method offers a versatile and comprehensive tool for investigating the interplay between material structure and ionic diffusion in SSEs. Implemented in the open-source CrySF package, our approach has been successfully applied to CMD and AIMD simulations across a range of promising SSE candidates, including $Li_7La_3Zr_2O_{12}$, $Li_{10}GeP_2S_{12}$, Li_6PS_5Br, Li_3PS_4, Li_3OCl, $LiGaO_2$, $LiMn(HCO_2)$, and $Li_2B_{12}H_{12}$. The results demonstrate strong alignment with both experimental and prior computational findings, underscoring the method's accuracy, versatility, and ability to illuminate complex correlations between structural features, ion mobility, and collective transport phenomena. Notably, we show that the mere existence of long, concerted diffusion chains, often seen as a defining trait of superionic conductors, is not by itself indicative of high IC. Factors such as the frequency of these chains, the diversity of sites visited, and the directional persistence of motion must all be considered.

References

[1] Deng, Z.; Zhu, Z.; Chu, I.-H.; Ong, S. P. *Chem. Mater.* **2017**, 29, 281–288.

[2] Zhang, Z.; Zou, Z.; Kaup, K.; Xiao, R.; Shi, S.; Avdeev, M.; Hu, Y.; Wang, D.; He, B.; Li, H.; Huang, X.; Nazar, L. F.; Chen, L. *Advanced Energy Materials* **2019**, 9, 902373.

[3] L.pez, C.; Rurali, R.; Cazorla, C. *J. Am. Chem. Soc.* **2024**, 146, 8269–8279. [4]He, X.; Zhu, Y.; Mo, Y. *Nat. Commun.* **2017**, 8, 15893.

[5] Kozinsky, B. In: *Handbook of Materials Modeling: Applications: Current and Emerging Materials*; Andreoni, W., Yip, S., Eds.; Springer International Publishing: Cham, 2018; 1–20.

[6] Richards, W. D.; Tsujimura, T.; Miara, L. J.; Wang, Y.; Kim, J. C.; Ong, S. P.; Uechi, I.; Suzuki, N.; Ceder, G. *Nat. Commun.* **2016**, 7, 11009.

[7] Kahle, L.; Musaelian, A.; Marzari, N.; Kozinsky, *Phys. Rev. Materials* **2019**, 3,055404.

Invited 25-035

Computational study of Solid Electrolyte Interphase in Lithium Batteries

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When lithium batteries are charged, a passivation layer, the so-called solid electrolyte interphase (SEI), forms at the anode/electrolyte interface. In ideal conditions, this passivation layer remains stable during cycling, allowing rapid lithium transport while acting as an electronic insulator. However, this interphase often exacerbates irreversible capacity loss associated with lithium depletion, increasing battery resistance. How to form a good SEI is crucial to the overall performance of the battery. In my talk, I will introduce how DFT and AIMD calculations can be used to understand the SEI formation mechanism and composition.[1-

3] Furthermore, I will explain the relationship between atomic charge and the core electron binding energy in XPS analysis to aid experimentalists in XPS curve fitting.[4]

References:

1. Liang-Ting Wu, Yu-Ting Zhan, Yu-Cheng Chiu, and Jyh-Chiang Jiang*, Small 2025 (21) 2503382.
2. Shih-Huang Pan, Santhanamoorthi Nachimuthu, Bing Joe Hwang, Gunther Brunklaus, and Jyh-Chiang Jiang*, Journal of Colloid and Interface Science 2023, 649, 804-814.
3. Lin, KY; Kuo, RT; Miyazaki, T; Hwang, BJ; Jiang, JC*, J. Energy Storage 2024, 88, 111674.
4. Liang-Ting Wu, Santhanamoorthi Nachimuthu, Daniel Brandell, Jyh-Chiang Jiang*, Batter. Supercaps 2022, 5, e202200088.

Invited 25-036

Stabilizing Lithium-Rich Cubic Garnet Electrolytes by Controlling Intrinsic Atomic Defects

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Safety concerns associated with flammable liquid electrolytes in lithium-ion batteries have intensified interest in all-solid-state batteries (ASSBs), which offer enhanced safety and higher energy density. Among various solid electrolytes, cubic garnet materials stabilized through aliovalent doping to introduce lithium vacancies exhibit high ionic conductivity and favorable chemical compatibility with lithium metal. However, these materials are susceptible to the formation of intrinsic atomic defects during high-temperature sintering, as well as to strain-induced phase transitions from the cubic to the tetragonal phase during mechanical processing. Such structural instabilities impede lithium-ion transport and facilitate undesirable interfacial reactions, thereby increasing the risk of short-circuiting.

In this study, we systematically investigate the formation and evolution of intrinsic atomic defects in cubic garnet-type $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$ (LLZTO) synthesized *via* conventional solid-state methods and subjected to mechanical processing under varying lithium contents. Furthermore, we introduce a new fabrication approach specifically designed to mitigate defect formation and preserve structural stability. Our findings underscore the critical importance of controlling lithium excess and mechanical strain during synthesis and processing to improve electrochemical performance. These insights advance our understanding of surface phase transitions in cubic garnet solid electrolytes and provide practical strategies for optimizing material properties while minimizing adverse interfacial reactions.

Keynote 25-010

Non-local interactions determine local structure and lithium diffusion in solid electrolytes

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Solid-state batteries, in which solid electrolytes (SEs) replace their liquid alternatives, promise high energy density and safety. However, understanding the relation between SE composition and properties, stemming from intricate interactions among constituent sublattices that involve non-local electronic and nuclear dynamics, remains a critical and unsolved challenge. Here, we evaluate electronic structure methods and demonstrate that a density-functional approach incorporating non-local and many-body effects in exchange-correlation interactions provides predictive results for the local structure and diffusion properties of SEs. Focusing on argyrodite SEs ($Li_{6\pm x}M_{1\pm y}S_{5\pm z}X_n$, LMSX; M = P, Ge, Si, Sn; X = Cl, Br, I), we explore their compositional landscape as a test case. The employed HSE06+MBDNL method unveils how the S/X site disorder dictates the diffusion of lithium by controlling the number and length of the diffusion pathways. Additionally, non-local exchange and van der Waals interactions precisely modulate the coupling between the framework lattice and mobile lithium ions, thereby influencing the migration barrier. Consequently, the interplay of non-local electronic interactions in the predictive design of Li-solid electrolytes – and likely many other functional materials – is emphasized. Finally, I discuss the promise of general-purpose machine-learned force fields (MLFFs) in accelerating *ab initio* accurate modelling of solid electrolytes and other functional materials.

Invited 25-037

Materials and Electrode design optimization for oxide based all-solid-state batteries

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Solid-state lithium batteries (SSLBs) are a promising candidate for safe, high-energy-density storage, with lithium lanthanum zirconium oxide (LLZO) standing out as a robust solid electrolyte due to its high ionic conductivity and chemical stability.

This talk will present a significantly improved processing strategy for LLZO. By reordering and optimizing the timeline of the fabrication steps, we have made tape-casting of LLZO not only feasible but also practical for large-scale production. A tailored material processing allows for a significant reduction in sintering temperature of LLZO, enabling a one-step production of fully ceramic cathode-separator half-cells for the first time.

The unique advantages of the tape-casting process also open up the possibilities for innovative processing and design strategies on a micro-scale. The introduction of a functional gradient within the mixed ceramic cathode, leads to improved capacity, better interface properties, and more efficient lithium transport, significantly improving the theoretical maximum thickness for complete usage of the active material in the cathode.

Furthermore, significant improvements for the production and performance of lithium-metal anodes will be presented. By introducing mixed metal anodes, the chemical and mechanical compatibility with the rigid LLZO interface in greatly improved. The self-formation of a nanostructured interface during the cycling of the battery reduces degradation of the cell performance significantly and thereby highlights the importance of interface engineering. Together, these results highlight the critical role of process control and structural design in advancing LLZO-based solid-state battery technologies.

Invited 25-038

Unveiling Structure-Ionic Conductivity Relationships in Sulfide and Halide Solid Electrolytes via Synchrotron X-ray Analysis

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There have been enormously increasing demands for developing next-generation Li-ion batteries with enhanced energy, power density, and safety features compared with the current state-of-the-art LIB technology. Such advances necessitate successfully developing and implementing the new cathode, anode, and (solid) electrolyte materials. In this regard, understanding the structure-property correlation of advanced battery materials has become a central aspect of battery research.

In particular, the development of highly conductive and (electro)chemically stable inorganic solid electrolytes (SEs) from cost-effective materials is essential for realizing all-solid-state batteries (ASSBs). A major challenge lies in elucidating the complex relationship between the atomic structure of SEs and their ionic conductivity. In this study, we investigate structure–ionic conductivity correlations in emerging sulfide- and halide-based SEs using a suite of synchrotron X-ray techniques, including X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS), and X-ray pair distribution function (PDF) analysis. Among these, PDF analysis is especially powerful in providing multiscale insights into atomic arrangements and disorder. We highlight its role in revealing how local structural features—such as site disordering, $[PS_4]^{3-}$ tetrahedral rotational dynamics in argyrodite frameworks, and interfacial/interphase conduction—affect the ionic transport properties of novel SEs. By probing these atomic-scale characteristics, our study aims to identify the key structural descriptors that control ionic conductivity and inform the rational design of next-generation solid electrolytes.

Invited 25-039

Na^+-ion conducting ceramics with superior performances

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The huge demand for delocalized energy storage due to the application of fluctuating energy sources leads to a need for low-cost devices available on a large scale and with high energy density. Sodium-based batteries show great potential in this field and have recently attracted extensive interest. Solid electrolytes (SEs) rather than liquid electrolytes display the advantages of non-leakage, non-volatilization, adaptability to temperature changes as well as compatible theoretical energy and power densities, which makes solid-state sodium batteries (SSNBs) potentially the batteries of the next generation. Plenty of Na-ion conducting SEs have been reported until now, such like ceramics, sulfides, boranes, chlorides, glasses, polymers, etc[1]. In this presentation, ceramics are specially addressed because of their high stability in normal atmosphere and low cost. Ceramics are defined as crystalline, non-metallic, inorganic materials which are usually formed by the application of sintering. Presently most of the reported ion conducting ceramics are oxides, including NaSICONs, $Na_5LnSi_4O_{12}$ (Ln = La-Lu and Y), beta-alumina, $Na_2X_2TeO_6$ (X = transition metal), Na_2O-TiO_2 based ceramics, etc[1]. The development of the former two types is a particular focus at our institute due to their excellent performance and relative ease of handling.

In the family of NaSICONs, $Na_{3.4}Zr_2Si_{2.4}P_{0.6}O_{12}$ (NZSP) ceramics are reported with unaverage total conductivity (σ_{total}) of 5×10^{-3} S cm^{-1} at 25 °C.[1-3] A remarkable Na dendrite-growth behavior along the ceramic surface rather than through the ceramic is also found for NZSP. *Operando* investigations and *in situ* SEM microelectrode experiments are conducted to reveal the Na plating mechanism. By covering the ceramic surface with sodium salt coatings, surface dendrite formation is prevented and the dendrite tolerance of Na | NZSP | Na symmetric cells is increased to a critical current density (CCD) of 14 mA cm^{-2} and galvanostatic cycling of 1 mA cm^{-2} / 1 mAh cm^{-2} (half cycle) is demonstrated for more than 1000 h.[4] It should be further noticed that compared to the extraordinary bulk conductivity (σ_{bulk}, 15mS cm^{-2} at 25 °C), the σ_{total} of NZSP is only fair due to micro-crack formation caused by the thermal expansion anisotropy. We further modify the grain boundaries of NZSP by adding 1-5 mol% $Na_3LaP_2O_8$ (NLP) or $LaNbO_4$ (LNO) to counteract the micro-crack formation. The σ_{total} of NZSP-NLP and

NZSP-LNO is increased to 7.1 and 9.3 mS cm^{-1} at 25 °C, respectively.[5,6] The dendrite tolerance of the modified NZSP is also increased to the CCD of 22 mA cm^{-2} and galvanostatic cycling at 10 mA cm^{-2}. For the cathode side, the inter-ceramic contact problems have also been solved by combining the infiltration of a porous electrolyte scaffold with precursor solution and *in situ* synthesis of electrode active material.[3,7] The resulting cells using $Na_3V_2P_3O_{12}$ (NVP), NZSP and Na as the positive electrode, electrolyte and negative electrode materials, respectively, can be stably operated with a capacity of 0.55 mAh cm^{-2} at high rate of 0.5 mA cm^{-2}. In addition, $Na_5LnSi_4O_{12}$-type ceramic solidi electrolytes are also investigated because of their promising ionic conductivity similar to NaSICONs. $Na_5YSi_4O_{12}$ (NYS) and $Na_{4.92}Y_{0.92}Zr_{0.08}Si_4O_{12}$ (NYZS) show σ_{total} of 1.0 mS cm^{-1} and 3.3 mS cm^{-1} at 25 °C [8,9], respectively. The CCD of NYZS against Na metal electrodes can reach 2.4 mA cm^{-2} [9]. The galvanostatic cycling time is more than 1000 h applying 1 mA cm^{-2} and 1 mAh cm^{-2}.[9] With positive sulfur composite electrode, a Na/NYS/S pouch cell can be operated with specific capacity of about 600 mAh g^{-1} for more than 100 cycles.[10]

References

[1]. Q. Ma, F. Tietz, *ChemElectroChem* 2020, *7*, 2693–2713

[2]. Q. Ma et al., *J. Mater. Chem. A,* 2019, *7*, 7766–7776

[3]. C.-L. Tsai et al., *J. Power Sources*. 2020, *476*, 228666

[4]. Q. Ma et al., *Adv. Energy Mater*., 2022, *12*, 2201680

[5]. L. Liu et al., *J. Power Sources* 2025, 626, 235773

[6]. L. Liu et al. *Adv. Energy Mater*. 2024, 14, 2404985

[7]. T. Lan et al. *Nano Energy,* 2019*, 65*, 104040

[8]. A. Yang et al., *Chem. Eng. J*., 2022, *435*, 134774

[9]. A. Yang et al., *eScience* 2023,*3*,100175

[10]. A. Yang et al., *Carbon Energy*, 2023, *5*, e371

Invited 25-040

Research on High-voltage Strategy of High-nickel Ternary Cathode Materials

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The structural and electrochemical degradation of high-nickel layered oxides ($LiNi_xCo_yMn_zO_2$, $x \geq 0.6$) under high-voltage operation remains a critical challenge for high-energy-density lithium-ion batteries. This study proposes a dual-doping strategy incorporating W^{6+} and Al^{3+} into $LiNi_{0.65}Co_{0.15}Mn_{0.20}O_2$ (NCM) to enhance cathode stability and performance. Multiscale characterization (in situ XRD, SEM/FIB-SEM/TEM, XPS/EPR) demonstrates that W-Al co-doping effectively mitigates cation disorder, stabilizes lattice oxygen, and suppresses microcrack propagation. Density functional theory calculations reveal the stabilization mechanism through bandgap reduction (0.6 eV), enhanced electronic conductivity, and strengthened metal-oxygen bonds. The optimized 1.5W-0.5Al-NCM cathode delivers exceptional electrochemical performance, including a high capacity of 205.95 mAh g^{-1} at 0.1C and remarkable rate capability (148.2 mAh g^{-1} at 15C), with outstanding cycling stability (122.17 mAh g^{-1} after 500 cycles at 1C, 2.5-4.5V).[1]

Furthermore, a novel W^{6+}- Nd^{3+} co-modification strategy establishes a triple mechanism of "surface passivation-lattice anchoring-conduction optimization," achieving 240.8 mAh g^{-1} at 0.1C (2.5-4.7V) with 60.26% retention after 800 cycles at 1C. The optimized cathode exhibits remarkable low-temperature performance (228.23 mAh g^{-1} at -20°C) and operates effectively across wide temperature (-20-60°C) and voltage (2.5-4.7V) ranges.

References

[1] H. Li, N. Wang, Y. Song, K. Dong, Y. Xing, M. Zhang, Y. Wang, Chemical Engineering Journal, 518 (2025).

Keynote 25-011

Active Learning for Battery Materials Discovery

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We have developed an active learning framework tailored for accelerated discovery of inorganic functional materials, including next-generation solid-state battery electrolytes. Traditional screening of vast chemical and structural design spaces via high-throughput experiments and first-principles simulations such as density functional theory (DFT) and ab initio molecular dynamics (AIMD) is prohibitively time-consuming and resource-intensive. To overcome this challenge, we integrate Bayesian optimization with metaheuristic algorithms—such as genetic algorithms, particle swarm optimization, and cuckoo search—into a unified active learning pipeline. This hybrid strategy not only accelerates computational workflows by efficiently navigating complex potential energy landscapes, but also optimizes experimental design by strategically selecting candidate compositions with high potential. Starting from sparse random initializations, our framework rapidly converges to previously unknown single-phase compounds exhibiting desirable target properties. By combining these algorithmic advances with closed-loop feedback, the system continuously refines its predictive models, enabling autonomous materials discovery without reliance on expert intuition. This approach has demonstrated broad utility across multiple classes of functional materials, offering a generalizable pathway for data-driven exploration and design in materials science.

Invited 25-041

Probing Ultrafast Dynamics in Battery Cathodes

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The transition to a sustainable energy economy relies on advanced battery technologies that offer high energy density, fast charging, and environmentally responsible materials. A critical factor influencing battery performance is the movement and localization of electronic charge. While these phenomena have been extensively studied at longer timescales, the ultrafast electronic and structural dynamics— remains limited, impeding insights into critical phenomena such as electron transfer, localization, and structural transformations in electrode materials like $LiMn_2O_4$ (LMO), despite their significant impact on battery performance [1][2].

In this talk, I will present our investigation into LMO, a model cathode material where strong electron-lattice interactions give rise to small Jahn-Teller (JT) polarons. LMO exhibits a ferrodistortive tetragonal ground state that undergoes a dynamic order-disorder transition around 290 K, where pseudorotations continuously reorient the JT axis. These fluctuations occur on timescales relevant to polaron formation, transport, and ion mobility. By combining AIMD simulations and Nudged Elastic Band (NEB) calculations, we show that the mechanistic interplay between JT dynamics and polaron transport critically governs the kinetics of charge transfer in LMO. I will also introduce our approach to analyzing these ultrafast phenomena using automated workflows, which are essential due to the large data volumes and the complexity of the computational techniques required to simulate the experimental observables. To simplify this task, we have recently developed PerQueue [3], a modular and dynamic Python-based workflow manager designed to facilitate complex autonomous workflows. PerQueue's modular architecture supports dynamic capabilities, allowing the definition of workflows upfront and representing them as acyclic dependency graphs—even when dynamic processes are involved. This feature is vital when integrating DFT simulations with machine learning or Monte Carlo techniques. Extending its application further, we demonstrate PerQueue's broader utility in self-driving laboratories and Materials Acceleration Platforms (MAPs), where its adaptability overcomes the limitations of static workflow managers and supports scalable, FAIR-compliant experimentation [4]. We aim to establish PerQueue as a foundational tool for managing complex, automated workflows that enable critical mechanistic insights for engineering improved battery materials with enhanced charge carrier mobility.

References

[1] Tygesen AS, Chang JH, García-Lastra JM, Phys Rev B. 2023, 108 (4), 045120.

[2] Nagle-Cocco LAV, Genreith-Schriever AR, Steele JMA, Tacconis C, Bocarsly JD, Mathon O, et al, J Am Chem Soc. 2024, 146 (43), 29560–74.

[3] Sjølin BH, Hansen WS, Morin-Martinez AA, Petersen MH, Rieger LH, Vegge T, et al, Digit Discov. 2024, 3 (9), 1832–41.

[4] Steensen SK, Butler PWV, Pedersen JR, Fisker-Bødker N, Vegge T, Chang JH, Castelli IE, Adv Intell Discov. 2025, Just Accepted.

Invited 25-042

Enabling Cloud-connected Labs of Future for Energy Materials

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A critical step in transitioning to a green future is the accelerated discovery and mobilization of high-performance materials for clean technologies. Clean energy transition by 2030 requires at least 10X acceleration for production-ready energy materials. In addition to resource intensive and insufficient success rates, current research infrastructures and practices take 10 to 20 years to advance a new material from discovery to commercialization.

The development of next-generation materials and components for energy storage technologies includes fabrication scale-up and integration with other cell components. R&D data assets are poorly utilized for developing new energy materials within emerging hydrogen technologies. The shortcoming in data utilization is largely driven by unstructured and complex data (type, category, quantity) from various experimental, synthesis, modelling and simulation sources. A unified data management approach, albeit a complex task, is essential for the discovery-to-device integration pipeline of new materials and components.

This presentation introduces opportunities and challenges in establishing a decentralised and adaptable future lab concept that speeds-up the development, integration, and innovation path for clean energy materials and technologies. In particular, the key challenges in availability of practical material-to-device data infrastructure within energy storage technologies are articulated. We address the gaps in availability of AI-ready data sources, AI-native predictive models, and the role of a robust, enterprise-grade cloud platform for accelerating development and early-prediction of materials properties and component performance.

General 25-011

Machine-learning-powered molecular dynamics simulations for accurate modelling of SEI materials in lithium-ion batteries

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The poorly controlled structure of the electrode/electrolyte interface remains a major bottleneck in advancing lithium-based battery performance.[1,2] In particular, the solid electrolyte interphase (SEI) formed on lithium-based anodes is critical to achieving high energy density, high coulombic efficiency, long cycle life, and improved safety. However, the SEI often undergoes significant morphological changes—such as cracking and continuous growth during lithium cycling, leading to capacity fade and eventual battery failure. Understanding the SEI remains a longstanding challenge due to its complex and largely unresolved atomic structure. Atomistic simulations, especially molecular dynamics (MD), offer valuable insights into SEI structure and evolution, but they require interatomic potentials that are both accurate and computationally efficient. While recent work has demonstrated the promise of machine learning-based force fields for battery materials—mainly focusing on electrolytes—their application to SEI modeling is still in its early stages, largely due to the lack of representative and reliable atomic datasets.[3] In this talk, we present a robust framework for developing machine learning interatomic potentials, using the moment tensor potential (MTP) trained on reference datasets derived from amorphous structures and density functional theory (DFT) calculations.[4] By integrating active learning loops, we efficiently sample the relevant configurational space and generate high-fidelity MD trajectories under battery operating conditions. Our trained MTP models accurately reproduce key structural properties—such as lattice constants, elastic moduli, and phonon spectra—as well as dynamic transport characteristics in SEI-relevant materials including Li_2CO_3, bulk Li, $LiPF_6$, and Li_2EDC. This machine learning-driven workflow provides a scalable and transferable approach for SEI modeling, enabling atomistic simulations with near-DFT accuracy.

References

[1] Tarascon, J.-M. & Armand, M. Issues and challenges facing rechargeable lithium batteries. Nature 414, 359–367 (2001).
[2] Peng, Y., Tamate, R. & Nishikawa, K. Review on Artificial Interphases for Lithium Metal Anodes: From a Mechanical Perspective. ChemElectroChem 11, (2024).
[3] Dajnowicz, S. et al. High-Dimensional Neural Network Potential for Liquid Electrolyte Simulations. J. Phys. Chem. B 126, 6271–6280 (2022).
[4] Li, W.-Q. & Ng, M.-F. Enabling accurate modelling of materials for solid electrolyte interphase in lithium-ion batteries using effective machine learning interatomic potentials. Manuscr. Prep. (2025).

Invited 25-043

Construction of a Robust Neural Network Potential for Large- Scale Molecular Dynamics Simulations of Polymer Electrolyte Membranes

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Machine learning interatomic potentials (MLIPs) have emerged as a powerful tool, enabling large-scale, long-duration molecular dynamics (MD) simulations with quantum mechanical accuracy. However, a significant challenge remains: MLIP-driven MD simulations often suffer from instabilities, a critical bottleneck for studying complex amorphous materials. Perfluorinated ionomers (Nafion), crucial components in fuel cells and electrochemical devices, are prime examples where robust potentials are essential for understanding their structure-property relationships and optimizing their performance. These materials demand stable, large-scale analysis to unravel the intricate interplay between morphology, hydration, and proton transport.

This study addresses the above-mentioned challenge by developing an exceptionally robust neural network potential (NNP), specifically a Deep Potential (DP) model, for Nafion membranes. We construct the DP model by iteratively expanding the training dataset through an active-learning scheme implemented in our NNP generator (GeNNIP4MD). Our strategy combines two key elements: sampling off-equilibrium structures via non-equilibrium MD simulations and a novel screening process in a 3D structural feature space that incorporates minimum interatomic distances. This approach significantly enhances the model's robustness, enabling stable MD simulations of large Nafion systems (10,000–20,000 atoms) for an extended duration of 31 ns across a wide range of hydration levels. The MD simulations using the developed DP model yield proton self-diffusion coefficients that show better agreement with experimental values across a wide hydration range compared to those from previous, smaller-scale ab initio MD simulations, offering valuable insights into the proton transport mechanisms within Nafion membranes.

Invited 25-044

Operando High-Temperature XAFS during Synthesis of $LiNiO_2$ Cathode Materials

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Nickel-rich lithium-containing layered oxides are used as cathode materials in lithium-ion batteries for automotive applications, and layered oxides with further higher Ni content are being developed for practical use. However, increasing the Ni content reduces the thermal stability and Li and Ni tend to mix at high temperatures during the synthesis process. To understand the Li/Ni mixing mechanism during synthesis of Ni-rich layered oxides, structural changes of starting materials or precursors were studied by using a high temperature in situ X-ray diffraction (XRD) technique during $LiNiO_2$ synthesis by Bianchini [1] and Weber [2]. Their results confirmed the loss of lithium and oxygen and the migration of Ni to Li layers above 700 °C. However, it is still unclear whether the driving force behind the Li/Ni mixing is the volatilization of lithium or the electrical state of Ni associated with oxygen release.

Here, operando high-temperature X-ray Absorption Fine Structure (XAFS) was performed during the synthesis of $LiNiO_2$ in an oxygen atmosphere to reveal the electrical structure of Ni at high temperatures. The effect of lithium volatilization was studied using the precursors with different lithium content. Preheated $LiNiO_2$ precursors were prepared by heating $LiOH{\cdot}H_2O$ and $Ni(OH)_2$ at 350 °C. To enable X-ray transmission, approximately 10 mg of precursor powder was formed into a very thin pellet less than 100 μm thick. Operando high-temperature Ni K-edge XAFS spectra were obtained by a transmission mode at Photon Factory (PF), High Energy Accelerator Research Organization (KEK), Japan while the pellet was heated to 900 °C and cooled to room temperature. The obtained operando spectra during synthesis of $LiNiO_2$ revealed a clear edge shift to the lower energy side corresponding to nickel reduction above 700 °C, regardless of whether the Li/Ni ratio is greater than 1. Since Li/Ni mixing was reported to start from 700 °C using operando X-ray diffraction,[1,2] the nickel reduction could be the cause of the Li/Ni mixing. The detailed synthesis reaction of $LiNiO_2$ is discussed in comparison with $LiCoO_2$ and doped $LiNiO_2$.

References

[1] M. Bianchini, J. Janek, *et al.*, *Angew. Chem., Int. Ed.*, 58, 10434 (2019).
[2] R. Weber, J. R. Dahn, *et al.*, *J. Electrochem. Soc.*, 167, 100501 (2020).

General 25-012

Factors affecting phase stability in layered oxide materials

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Sodium ion batteries (SIBs) are an attractive alternative to Lithium-ion batteries (LIBs) due to the abundance and low cost of Na. Layered Li transition metal oxides (Li_xTMO_2), commonly used as cathode materials for LIBs, exist only in the octahedral (O) stacking structure, while layered Na_xTMO_2 of SIBs and K_xTMO_2 cathodes of KIBs can exist in the prismatic (P) phase as well. This may lead to design challenges as well as unfavourable phase transitions during cycling.

In this study, the mechanism of P2 phase formation is investigated using electrostatics and density functional theory (DFT) calculations. Electrostatics calculations show the O3 phase becomes more energetically favoured, when compared with P2, with decreasing interlayer distance. In particular, for interlayer distances corresponding to Na_xTMO_2, P2 became favoured in between approximately 0.45 and 0.85 Na concentration. To support this finding, the DFT energies for $NaMnO_2$ and $NaCoO_2$ with several Na concentrations were calculated, revealing a similar trend, differing in that the energy difference between P2 and O3 phase was much smaller at small Na concentration. However, this window of P2 stability widens when the TM experiences localization of charges (such as the case with Mn). At interlayer distances in the range of those for K_xTMO_2, the Coulomb energies confirm that P2-phase is more stable for the majority of the K concentration range.

Separating the available alkali metal sites of the P2 structure into face-sharing and edge-sharing sublattices shows that a combination of both is occupied for the most energetically favoured Na-ion arrangement. Furthermore, breaking down the Ewald energy into pair-interaction components for Na_xCoO_2 (Na-Na, Na-O, Na-Co, Co-O) shows that at interlayer distances approximately larger than 3.2Å the Na-Na electrostatic interaction dominates and favours the P2 phase, as the P2 structure has a higher number of allowed Na sites than O3. Additionally, DFT calculated radial distribution functions for $Na_{0.67}MnO_2$ and $Na_{0.67}NiO_2$ show two bond lengths for both Mn-O and Ni-O, indicative of Jahn-Teller distortion. Magnetic moments for $Na_{0.67}MnO_2$ and $Na_{0.67}CoO_2$ calculated with DFT-PBE reveal a delocalized distribution of charges across the Co atoms, but the Mn atoms exhibit localised charges. We conclude that P2 phase formation is influenced by interlayer separation (driven by charge-carrier size), disproportion of TM charges, and the combination of prismatic site occupation. All of these factors could be determined using Electrostatics calculation.

Invited 25-045

Advancing High-energy Density Layered Materials for Sodium-ion Batteries: from Basic Principles to Industrialization

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Branded with low cost and a high degree of safety, with an ambitious aim of substituting lithium-ion batteries in many fields, sodium-ion batteries have received fervid attention in recent years after being dormant for decades. The electrochemical performance of layered cathode materials is highly contingent on the building elements and microstructures. This talk will discuss our advancements in promoting low-cost and high-energy density layered materials for commercial Sodium-ion batteries covering basic principles, materials mass production as well as the design of practical pouch cells with over 160 Wh/kg energy density.

References

[1] M. Li and B. Xiao* et al., Nat. Commun., 16 (2025) 2010
[2] T. Huang and B. Xiao* et al., J. Am. Chem. Soc., (2025)
[3] G. Pang and B. Xiao* et al., Adv. Funct. Mater., (2025) 2505824
[4] Z. Guan and B. Xiao* et al., Mater. Today, 87 (2025) 176
[5] M. Li and B. Xiao* et al., Energy Environ. Sci., 17 (2024) 7058
[6] X. He and B. Xiao* et al., Nano-Micro Lett., 17 (2025) 45
[7] B. Xiao* and X. Li et al., Adv. Mater., 36 13 (2024) 2308380
[8] M. Li, H. Zhuo, B. Xiao* et al., Carbon Energy, (2024) e545
[9] M. Li, H. Zhuo, B. Xiao* et al., Nano Energy, 123 (2024) 109375
[10] C. Li, K. Wang, B. Xiao* et al., ACS Appl. Mater. Inter.,16, 35 (2024) 46216
[11] X. Yang, L. Zhang, B. Xiao* et al., ACS Appl. Mater. Inter., 16, 31 (2024) 40805
[12] K. Wang and B. Xiao* et al., *Adv. Funct. Mater.*, (2023) 2212607

General 25-013

A Semi-empirical Descriptor for Open Circuit Voltage

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Layered transition metal oxides (TMO) are widely used as cathode materials in Na/Li batteries. The open-circuit voltage (OCV), which determines the energy density (together with capacity), is among the key physical and chemical factors influencing the performance of cathodes. The voltage profile is influenced by the formation energy of intermediate phases during cycling. From a theoretical perspective, the formation energy (and voltage) is defined as total energy differences between intermediate phases. Therefore, an accurate prediction of total energy difference is crucial for the prediction of OCV.

In this work, we present a theoretical framework that decomposes the total energy difference between adjacent phases of a given TMO into distinct, physically meaningful contributions. Specifically, we express the energy difference in terms of parameters that are accessible, either computationally less demanding than full DFT calculations or directly available from experimental databases. From these parameters, we define a composition-dependent potential term that enables the calculation of voltage profiles across a range of TMO compositions.

This approach offers a computationally efficient method for predicting the open-circuit voltage (OCV) across a wide range of transition metal oxides (TMOs). The significantly reduced computational cost enables the screening of a much broader configuration space of intermediate compositions during charge-discharge cycles, thereby improving the resolution and accuracy of predicted voltage plateaus. Moreover, the method facilitates the rapid evaluation of high-resolution formation energy landscapes, which are typically beyond the practical scope of conventional DFT calculations. This method is well-suited for high-throughput studies, where rapid and reliable evaluation of key parameters is essential. We validated our framework by successfully reproducing unrelaxed DFT-calculated voltage plateaus for 14 different TMO compositions, achieving reasonable agreement with available experimental voltage data.

General 25-014

Digital Twin-guided Design of Air Electrode Structures for Enhanced Metal-air Battery Performance

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Metal–air batteries have been gaining attention as next-generation energy storage systems due to their high theoretical energy densities, enabled by the use of ambient oxygen as a redox reactant. This characteristic allows them to surpass conventional lithium-ion batteries in specific energy density, making them promising candidates for applications such as electric vehicles and energy storage systems, where maximizing energy within constrained volume and weight is critical. However, their commercialization remains hindered by sluggish oxygen reduction and evolution kinetics at the air electrode, leading to limited capacity and low round-trip efficiency. While extensive efforts have been made to improve catalytic materials to enhance electrochemical reactivity, relatively little attention has been paid to the structural design of the air electrode. This structure critically determines the formation of triple phase boundary and governs mass transport properties.

In this study, we present a digital twin-driven approach to investigate the effect of structural design parameters on the electrochemical performance of air electrodes. An electrochemical model for metal–air batteries was developed to simulate discharge behavior under realistic operating conditions. Using this model, we systematically analyzed the influence of key structural parameters on oxygen transport and reaction kinetics. The results revealed that optimizing the internal architecture of the air electrode can enhance discharge capacity and reduce overpotential. Based on these insights, we propose a rational structural design strategy to improve the catalyst utilization in metal–air battery systems.

Poster 25-001

Constructing a conductive and sodiophilic nucleation layer towards efficient sodium plating and stripping

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Benefiting from significant improvements in gravimetric and volumetric energy densities compared to conventional ones, recently, anode-free alkaline metal batteries (AFAMBs) have been extensively investigated. When employing Cu or Al foil as a current collector in the anode, however, it typically suffers from the obvious increases in the nucleation barrier and overpotential, and non-uniform plating/stripping. Eventually, they cause poor Coulombic efficiency and limited cyclability of AFAMBs. Accordingly, searching for a facile and efficient strategy to address the afore-mentioned issues is of significance and emergently desirable as well. Herein, 10 μm of the nucleation layer coated on Al (NL-Al) was designed as an alternative anode to explore the stability of sodium plating/stripping in an ether-based electrolyte. Upon the testing conditions of 0.5 mA/cm^2 and 1 mAh/cm^2, the initial nucleation and growth potentials of NL-Al were -25.0 mV and -8.1 mV (vs. Na/Na$^+$), respectively. Encouragingly, its initial Coulombic efficiency of NL-Al was also achieved at 94.6 %. The initial nucleation and growth potentials were not dramatically raised (i.e., -69.9 mV and -52.0 mV (vs. Na/Na$^+$) even with a gradual increase in the current density to 5 mA/cm^2, while maintaining 98.8 % of Coulombic efficiency. The positive results disclosed here can be attributed to enhanced electronic conductivity and favorable sodiophilicity of NL, suggesting its potential application towards anode-free sodium metal batteries.

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Poster 25-002

Influence of Oxygen Vacancies on Defect Dynamics, Structural Integrity, and Electrochemical Performance in Layered NCM Cathode Materials

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Layered transition metal oxide cathodes are essential for high-energy-density lithium-ion batteries, offering both high capacity and power capability. Among them, nickel–cobalt–manganese (NCM) materials are particularly sensitive to synthesis conditions, especially oxygen partial pressure, which critically affects structural integrity, defect chemistry, and electrochemical performance. Here, we systematically investigate the impact of oxygen pressure during synthesis on NCM stability and functionality. NCM samples were prepared under controlled oxygen pressures and analyzed using high-resolution powder diffraction (HRPD), in situ X-ray diffraction (XRD), high-energy-resolution fluorescence-detected X-ray absorption spectroscopy (HERFD-XAS), and density functional theory (DFT) calculations. Low oxygen pressure induced pronounced phase transformations, increased Li/Ni antisite defects, and reduced specific capacity. HERFD-XAS revealed that oxygen-deficient samples exhibit lower Ni oxidation states, impairing electrochemical activity. DFT results confirmed that high oxygen pressure suppresses oxygen vacancy formation, whereas low oxygen pressure promotes vacancies that stabilize Li/Ni disorder and accelerate structural degradation. These findings establish a direct mechanistic link between oxygen-pressure-driven defect formation and performance deterioration, highlighting the importance of precise oxygen control for developing robust, high-performance NCM cathodes.

Poster 25-003

Fluorine-Free Epoxy Binder Design for High-Energy-Density Lithium-Ion Battery

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With the rapid expansion of electric vehicle adoption, increasing the energy density of lithium-ion batteries has become a critical challenge. To achieve this, the development of high-capacity cathode materials and thick (high-loading) electrodes is gaining significant attention. In line with this technological trend, securing the mechanical cohesion between active materials and strong adhesion to the current collector has emerged as a key requirement for electrode design. However, conventional fluorinated binders such as polyvinylidene fluoride (PVDF) rely on van der Waals interactions for adhesion, resulting in limited mechanical strength. This often leads to structural instability, including cracking and delamination, particularly in thick electrodes. Furthermore, fluorinated materials like PVDF fall under the category of per- and polyfluoroalkyl substances (PFAS), which are environmentally persistent and bioaccumulative, and are thus increasingly subject to global regulatory restrictions. Consequently, there is a growing need for next-generation binders that are fluorine-free (F- and PFAS-free), while offering high mechanical strength, chemical resistance, and thermal stability. In this study, we designed an epoxy-based binder with excellent mechanical properties and electrochemical stability, and evaluated its applicability in cathode electrodes for improving structural integrity and enabling environmentally responsible battery manufacturing processes.

Poster 25-004

Dry-Processed Thick Electrodes for Aqueous Zinc–Iodine Batteries with Enhanced Energy Density

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Aqueous zinc–iodine batteries (ZIBs) have emerged as promising candidates for next-generation energy storage systems due to their low cost, high theoretical capacity, and inherent safety. However, their commercialization remains limited by insufficient energy density and high production costs.

To address these limitations, we developed a dry electrode fabrication strategy to produce thick cathodes. This solvent-free method effectively suppresses the migration of binders and conductive additives, enabling higher active material loading within a fixed cell volume and thereby improving energy density. It also reduces the use of passive components such as separators and current collectors, contributing to improved cell-level efficiency. This benefit is particularly relevant for ZIBs, where titanium foil is typically used as the current collector instead of aluminum due to its superior corrosion resistance. However, its higher density (Al: 2.7 g/cm^3; Ti: 4.5 g/cm^3) and lower electrical conductivity (Al: 3.77×10^7 S/m; Ti: 0.24×10^7 S/m) make its excessive use detrimental to both gravimetric performance and cost. Implementing thick electrodes mitigates this issue by reducing the relative amount of current collectors required per unit capacity, highlighting the importance of thick electrode design in achieving high-performance and lightweight ZIBs.

In this work, porous carbon was further incorporated into the electrode structure to enhance electronic conductivity and facilitate high iodine loading. Free-standing electrodes were fabricated, achieving an areal capacity of 5.2 mAh/cm^2 at 1C. These findings highlight the potential of dry-processed ZIBs as a sustainable and scalable alternative to conventional slurry-cast systems, offering enhanced electrochemical performance and reduced environmental impact.

Poster 25-005

Residual NMP-Induced Degradation in Sodium-ion Batteries: Benefits of Dry Electrode Processing

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In this study, we investigate the impact of residual N-methyl-2-pyrrolidone (NMP) in wet-processed electrodes on the electrochemical and mechanical performance of sodium-ion batteries utilizing layered oxide cathodes. A comparative analysis is conducted between electrodes fabricated via traditional wet coating and emerging dry coating techniques, particularly under high areal loading conditions.

Gas chromatography–mass spectrometry (GC/MS) confirms the incomplete removal of NMP in wet-processed electrodes, even after standard drying procedures. Electrochemical testing reveals that the presence of residual NMP leads to increased cell resistance and inferior cycling stability compared to dry-coated electrodes. Furthermore, cross-sectional SEM imaging indicates severe structural damage and electrode cracking in wet-processed samples, while dry-coated electrodes maintain structural integrity. Additional electrochemical impedance spectroscopy (EIS) and X-ray photoelectron spectroscopy (XPS) analyses suggest that residual NMP alters solid–electrolyte interphase (SEI) formation and promotes unstable surface reactions. High-loading electrode tests demonstrate that the dry process offers superior performance and mechanical robustness, making it more favorable for practical applications.

This work highlights the critical influence of solvent residues on cell reliability and presents dry electrode fabrication as a promising strategy to enable high-performance, sustainable sodium-ion batteries.

Keyword: Sodium-ion batteries, Residual NMP, Dry electrode fabrication

Poster 25-006

Dual-salt concentration control in an in-situ polymerized gel polymer electrolyte for high-performance lithium-ion batteries

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In recent years, quasi-solid-state lithium-ion batteries (QSSLIBs) have attracted attention as a promising approach to improving battery safety. Among various quasi-solid-state electrolytes, gel polymer electrolytes (GPEs), which trap liquid solvents within a polymer matrix, offer enhanced safety by mitigating electrolyte leakage and retain high ionic conductivity. However, the electrochemical performance of QSSLIBs remains limited, primarily due to the poor interfacial contact between the electrolyte and electrode. To address this issue, a dual-salt GPE was fabricated via in-situ polymerization to enhance interfacial compatibility and electrochemical performance.

The GPE was synthesized by incorporating two lithium salts ($LiPF_6$ and LiTFSI) into a DOL/EC solvent, followed by in-situ polymerization at room temperature. It was found that the concentration of both salts significantly influences the interfacial compatibility and structural properties of the resulting GPE. The optimized GPE exhibited a high lithium-ion transference number (0.63), a wide electrochemical stability window (~5.0 V), and stable lithium stripping/plating behavior over 2000 hours at a current density of 1.0 mA cm^{-2}. Furthermore, compared to liquid electrolytes, $LiFePO_4$ (LFP) and $LiNi_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) cells assembled with GPEs both demonstrated excellent cycling performance. Specifically, the LFP cell and NCM811 cell maintained capacity retention of ~100% and 68% after 500 and 200 cycles, respectively. In summary, this work presents an electrolyte design strategy of dual-salt GPEs, which effectively enhances electrode/electrolyte interfacial contact, suppresses lithium dendrite formation, and further improves battery safety and electrochemical performance.

Poster 25-007

Designing current collector interfaces for high-performance dry-processed cathodes

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Lithium-ion batteries (LIBs) are widely used in electric vehicles and energy storage systems. As demand grows for energy density, sustainability, and cost efficiency, thick electrodes have gained attention as an effective strategy to improve cell-level performance. However, slurry-based fabrication of thick electrodes involves toxic solvents, environmental issues, and binder migration, resulting in structural inhomogeneity and poor ionic transport. Dry electrode processing offers a practical alternative by eliminating solvents, reducing energy and cost, suppressing migration, and enabling scalable roll-to-roll production.

To further enhance performance, interfacial design between the electrode and current collector is essential. Despite its critical role in electron transport, mechanical support, and interfacial resistance, the current collector has received limited attention. These functions become more important in thick electrodes with high active material loading, where interfacial adhesion and stability strongly affect electrochemical behavior.

In this study, a single-walled carbon nanotube (SWCNT) coating was applied to an aluminum current collector as an interfacial layer for fabricating a dry-processed cathode. The electrode exhibited higher initial discharge capacity and improved cycle life and rate capability. Interfacial resistance was reduced by approximately 40%, attributed to more efficient electron transport across the well-connected interface. **The SWCNT layer improved interfacial contact and wettability, leading to stronger adhesion, more stable electrode structure, and lower interfacial resistance.**

Poster 25-008

Optimization of Dry-Processed NCM Cathodes in Lithium Rechargeable Batteries: Effect of Binder Type on Electrochemical Performance

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In lithium-ion battery electrode fabrication, binders critically influence electrochemical performance, structural stability, and adhesion. With increasing regulatory restrictions on PFAS (per- and polyfluoroalkyl substances) contained in fluorinated binders such as PVDF (polyvinylidene fluoride) and PTFE (polytetrafluoroethylene), environmental concerns have grown, highlighting the need for the development of fluorine-free alternative binders. However, the behavior and compatibility of such alternative binders under dry processing conditions have not been sufficiently investigated, and systematic comparative studies are still lacking.

Therefore, this study addresses this gap by evaluating the performance and applicability of various binders in dry-processed cathodes. Specifically, it investigates how different binder chemistries influence the structural integrity and electrochemical behavior of dry-processed NCM ($LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$) cathodes. The binders used in this study include PVDF, PTFE, and a fluorine-free hydrocarbon-based polymer. The hydrocarbon-based binder was selected for its cohesive characteristics without the use of solvents and its environmental friendliness, while the fluorinated binders were used as reference standards to assess the impact of fluorine-free substitution on performance.

All electrodes were fabricated under identical mixing and pressing conditions to ensure consistent and fair comparison. Prior to the binder comparison, dry processing conditions were optimized by adjusting the pressing temperature stepwise. The optimal pressing temperature was selected based on a comprehensive assessment of electrode structure and electrochemical performance. To evaluate the electrochemical implications of each binder type, Electrochemical properties were evaluated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), and high-rate charge/discharge performance and electrode stability were comprehensively analyzed under various C-rate conditions and long-term cycling tests.

Keyword: Lithium batteries, binder, polyfluoroalkyl substances, hydrocarbon polymer

Poster 25-009

Extraction of Mn by precipitation from black mass in waste lithium battery recycling process

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This study proposes a precipitation-based recycling process to efficiently recover valuable metals from used lithium rechargeable batteries. The amount of waste batteries has increased in recent years due to the growing use of electric vehicles and portable electronic devices. This has led to environmental pollution and the depletion of limited resources. These batteries contain large amounts of valuable and rare metals, such as lithium, cobalt, nickel and manganese. Effectively recovering these metals is essential to creating economic value and establishing a sustainable resource circulation system.

This study focuses on selectively precipitating desired metals from waste batteries through a process involving shredding, electrolysis, and the addition of a precipitant. During precipitation, a precipitating agent ionizes the valuable metals in the solution phase. Then, specific metal ions are precipitated and separated into compounds by controlling conditions such as pH, temperature and so on. This study focuses particularly on deriving the optimal conditions for the selective recovery of manganese.

This research provides an economical, environmentally friendly alternative to existing, complex, energy-consuming processes for recycling waste batteries. The precipitation method offers advantages such as easy process control and high-purity metal recovery at a relatively low cost. The results of this study are expected to improve the recovery rate of valuable metals from waste batteries, increase the efficiency of the recycling process, and provide important fundamental data for developing waste battery recycling technology.

Keyword: Waste battery recycling, precipitation method, metal recovery, manganese

Poster 25-010

Preparation of C-coated Si powders from Si kerf and biomass using microwave heating for lithium ion batteries

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The performance of LIBs is primarily determined by the properties of the cathode and anode materials, with the anode playing a critical role in determining the overall capacity, lifespan, and safety of the battery. Currently, commercial anode materials are predominantly based on graphite, which has been widely adopted due to its excellent stability and low cost. However, the theoretical capacity of graphite is limited to 372 mAh/g, which poses a challenge in meeting the growing demand for high-energy-density batteries. Among various alternatives, silicon (Si) has attracted significant attention as a promising anode material. Silicon offers a remarkably high theoretical capacity of around 4,200 mAh/g—more than ten times that of graphite—as well as a low operating potential, natural abundance, low cost, and environmental friendliness. However, Si anodes face major challenges. During repeated lithiation and delithiation processes, Si particles undergo a volumetric expansion of up to ~300%, leading to particle fracture and continuous growth of the solid electrolyte interphase (SEI). These phenomena severely degrade electrical conductivity, ion transport, and overall efficiency, ultimately resulting in reduced capacity and cycle life. Therefore, overcoming these limitations is essential for the practical application of Si-based anodes.

In this study, carbon-coated silicon powder (C@Si) was synthesized by coating silicon kerf—a byproduct of the silicon solar cell manufacturing process—with 15 wt% lignin dissolved in DMSO, followed by microwave-assisted carbonization. The entire carbonization process was completed within 2 minutes, significantly reducing the reaction time compared to conventional thermal treatments. The electrochemical performance of the resulting C@Si anode material showed an initial discharge capacity of 520 mAh/g at a 5C rate and maintained stable capacity retention over 30 cycles. This study demonstrates an effective and eco-friendly strategy for developing high-performance anode materials by recycling industrial wastes such as silicon kerf and lignin, while also dramatically shortening the carbonization time using microwave processing.

Keyword: Anode, silicon, silicon kerf, lignin, lithium batteries

Poster 25-011

Surface Modification of OLO Cathodes via Dry-Coated Nano-LFP for Thermal and Structural Reinforcement

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The rising demand for high-energy-density lithium-ion batteries (LIBs) in electric vehicles and electronics has accelerated the search for cost-effective and high-capacity cathode materials. Among these, over-lithiated layered oxides (OLOs), characterized by high Mn content and the absence of Co, offer attractive features such as low cost and specific capacities exceeding 250 mAh g^{-1}. However, extracting additional lithium from the Li_2MnO_3 component requires charging above 4.4 V, which induces severe oxidative stress. This leads to side reactions, phase transitions, and thermal instability, limiting practical application.

To mitigate these issues, we applied nano-sized lithium iron phosphate (LFP) particles onto the OLO surface via a dry-coating technique. Compared to conventional wet coating, the dry process is solvent-free, environmentally friendly, and industrially scalable. The nano-LFP layer acts as a physical and chemical barrier, minimizing surface degradation and stabilizing the electrode–electrolyte interface under high-voltage conditions.

Through transmission electron microscopy (TEM), we observed that the LFP layer effectively suppresses the transition from layered to spinel phases during cycling. Differential scanning calorimetry (DSC) confirmed improved thermal stability, with reduced exothermic heat generation. Furthermore, electrochemical testing demonstrated enhanced cycle retention and reduced capacity fading, validating the stabilizing role of dry-coated LFP.

These findings demonstrate that dry-coated nano-LFP not only improves thermal and structural stability but also extends the cycle life of OLO cathodes under demanding conditions. This study highlights the potential of dry surface engineering as a viable route for improving high-voltage cathode materials, offering a path toward safer and more durable next-generation LIBs.

Keywords : Lithium ion batteries, Over-lithiated layered oxide, Lithium iron phosphate, Dry coating

Poster 25-012

$AgNO_3$-Preplanted Li Metal Powder Electrode: Preliminary Formation of Lithiophilic Ag and a Li_3N-rich Solid Electrolyte Interphase

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Li metal powders (LMPs) are beneficial to fabricating thin and large-area Li electrodes for Li metal batteries (LMBs) owing to slurry coating-based manufacturing and facile impregnation of functional additives. 3D structure of LMP-based composites can alleviate the local current density even at a higher current. However, non-uniform nucleation and growth persist as barriers to guaranteeing both the performance and safety of LMBs. Here, we report an $AgNO_3$-preplanted LMP electrode for securing long stable cycling of LMBs. During pre-mixing the LMP slurry with $AgNO_3$ additive, it can chemically form lithiophilic Ag that can offer favorable nucleation sites throughout the LMP surface. At the same time, nitrates can help enrich a highly conductive, robust Li_3N into solid electrolyte interphase (SEI). Pre-planting $AgNO_3$ into a 40 μm-thick LMP electrode reinforced the cycling stability up to 500 cycles with 86.8 % capacity retention at 1C/3C charging/discharging rates and allowed superior rate capability up to 30C.

Poster 25-013

Performance Enhancement of Lithium–Sulfur Batteries via Polysulfide Adsorption Using a Fe_2P@MWCNT Interlayer

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Lithium–sulfur (Li–S) batteries have emerged as a promising next-generation energy storage technology owing to their high theoretical capacity (1675 mAh/g), exceptional energy density (~2500 Wh/kg), cost-effectiveness, and environmental sustainability driven by the natural abundance of sulfur. Despite these advantages, the practical implementation of Li–S batteries is hindered by several inherent challenges, including the intrinsically low electrical conductivity of sulfur (~10^{-3} S/cm), the dissolution and migration of lithium polysulfides (Li_2S_x, $x = 4–8$) that induce the shuttle effect, pronounced volume expansion (~80%) during cycling, and the instability of the lithium metal anode. To overcome these issues, we designed and fabricated an Fe_2P-embedded porous multi-walled carbon nanotube (Fe_2P@MWCNT) interlayer, which was coated onto a polyethylene separator via vacuum drying at 50 °C. The porous MWCNT network facilitates enhanced electrolyte infiltration and provides continuous ionic/electronic pathways, while the uniformly distributed Fe_2P nanoparticles serve dual functions: improving electrical conductivity and catalyzing the redox conversion of polysulfides. Furthermore, the biphasic Fe_2P structure exhibits strong chemical affinity toward lithium polysulfides, effectively anchoring them and mitigating the shuttle phenomenon. As a result, the Li–S cell incorporating the Fe_2P@MWCNT interlayer demonstrated a high initial discharge capacity, remarkable cycling stability, and outstanding rate capability. Electrochemical impedance spectroscopy confirmed a reduction in charge-transfer resistance and improved interfacial reaction kinetics. These findings underscore the potential of Fe_2P@MWCNT interlayers as a viable and scalable strategy to address the fundamental limitations of Li–S batteries and promote the advancement of high-performance sulfur-based energy storage systems.

Poster 25-0014

Poled BaTiO3/Lithiated-SPEEK coated separator for improved safety and electrochemical performance in lithium metal batteries

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Separators prevent direct contact between the electrodes and are essential for the safe operation of lithium-metal batteries, but commercial polyolefin separators suffer from low electrolyte wettability and poor thermal stability, leading to shrinkage and internal short circuits at high temperatures. Moreover, their limited electrolyte affinity results in suboptimal electrochemical performance. In this study, we fabricated a functional separator by coating a polyethylene (PE) substrate with ferroelectric $BaTiO_3$ (BTO) nanoparticles and lithiated sulfonated poly(ether ether ketone) (LSP). The BTO dipoles were aligned via a poling process, resulting in a poled-$BaTiO_3$ /LSP (PBTO/LSP) coated separator. The PBTO/LSP coated separator demonstrates improved electrolyte wettability, thermal stability, and higher ionic conductivity compared to a bare PE separator. Furthermore, the lithiated sulfonic acid ($Li–SO_3$) groups in LSP contribute to an increased lithium-ion transference number (t_{Li^+}) by limiting anion mobility, thereby promoting a uniform Li^+ flux. This separator exhibited a lithium-ion conductivity of 0.230 mS cm^{-1}, higher than that of the bare PE separator with 0.198 mS cm^{-1}. Within the coated layer, the $Li–SO_3$ groups promote a uniform Li^+ flux, and the PBTO layer suppresses lithium dendrite growth. In NCM811/Li cells with PBTO/LSP separator achieved and excellent dischargd capacity of 192.86 mA h g^{-1} and maintained a stable discharge capacity up to 200 cycles.

Poster 25-015

Understanding the Role of Electrolyte in Lithium–Sulfur Batteries

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Lithium–sulfur (Li–S) batteries have emerged as a promising next-generation energy storage system owing to their high theoretical energy density and cost-effective sulfur cathodes. However, their practical application is hindered by polysulfide dissolution and migration, leading to the shuttle effect and rapid capacity fading. The electrolyte plays a critical role in governing polysulfide solubility, transport behavior, and interfacial stability, directly impacting both sulfur utilization and cell energy density. In this study, we aim to identify and understand the influence of electrolyte composition and electrolyte-to-sulfur (E/S) ratio on Li–S battery performance. By systematically varying these parameters, we investigate their effect on capacity retention, Coulombic efficiency, and rate capability, with a particular focus on balancing polysulfide shuttle suppression and electrochemical kinetics. We expect these results to provide fundamental insights into electrolyte design strategies for achieving high capacity and stable cycling in Li–S batteries. Further details will be presented in this poster.

Poster 25-016

Catalytic Interface Design with MoS_2 for High-Performance Lithium-Sulfur Batteries

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Lithium–sulfur (Li–S) batteries are considered one of the most promising next-generation energy storage systems due to their high theoretical energy density and the natural abundance of sulfur. However, the commercialization of Li–S batteries is hindered by the shuttle effect of lithium polysulfides (LiPSs) and the poor electrical conductivity of sulfur and its discharge products, which lead to rapid capacity fading and limited rate performance. Thus, effective strategies to suppress LiPS migration and enhance redox kinetics are critically needed.

In this study, molybdenum disulfide (MoS_2) was introduced as a dual-function catalyst to enhance LiPS adsorption and accelerate redox reactions. MoS_2 provides active Mo and S sites for chemical interaction with Li^+ ions, while its 1T metallic phase offers improved electrical conductivity and faster electron transfer. To maximize catalytic performance, the MoS_2 structure was carefully controlled in terms of morphology (nano-flower for high surface area), particle size (tens of nanometers), and phase (high 1T content). Nano- MoS_2 was synthesized via a hydrothermal method in the presence of MWCNTs, forming a MoS_2/MWCNT composite. Sulfur was then incorporated by ball milling and melt diffusion to produce S@MoS_2/MWCNT, which was used to fabricate cathodes for electrochemical evaluation. Further improvements will be pursued by introducing acid-treated MWCNTs for better interfacial bonding and doping the MoS_2 composite with elements such as Co or Se to enhance LiPS adsorption and redox kinetics.

Poster 25-017

Ion-Conductive LLZTO Lithium Composites for Uniform Li Deposition and Enhanced Stability in Li-Metal Batteries

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Lithium metal batteries (LMBs) have been regarded as one of the most promising next-generation energy storage devices due to their ultrahigh theoretical specific capacity (3860 mAh g^{-1}), low density (0.53 g cm^{-3}), and the lowest redox potential (-3.04 V vs. SHE). Despite these remarkable advantages, the practical application of LMBs is still hindered by the intrinsic instability of the Li metal-electrolyte interface, resulting in Li dendrite growth and the formation of inactive "dead Li."

In this study, we propose a novel Li composite anode in which $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ (LLZTO) particles are uniformly dispersed within a metallic Li matrix via a simple mechanical kneading process. The embedded LLZTO particles have higher ionic conductivity (~10^{-3} S cm^{-1}) than the solid electrolyte interphase (SEI) layer (~10^{-6} S cm^{-1}) and function as efficient ion-conducting pathways, enabling uniform Li-ion flux and effectively suppressing dendritic Li growth. As a result, the Li/LLZTO-20 composites, optimally containing 20 wt% LLZTO relative to the Li metal, exhibited significantly reduced nucleation overpotential and excellent electrochemical cycling stability in symmetric cell tests. Moreover, full-cell tests employing the Li/LLZTO-20 anode show markedly enhanced cycling performance compared to cells using bare Li.

Poster 25-018

Controlled Nitrogen Doping in Vertically Aligned Carbon Nanotubes for Lithium–Sulfur Battery Anodes

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Lithium–sulfur (Li–S) batteries have emerged as promising next-generation energy storage systems, attributed to the high theoretical capacity of sulfur (1675 mAh g^{-1}), its natural abundance, and low cost. Despite these advantages, the practical implementation of Li–S batteries remains limited by critical challenges associated with lithium metal anodes, such as dendritic lithium growth, unstable electrode–electrolyte interfaces, and poor cycling stability. In this study, nitrogen-doped vertically aligned carbon nanotubes (N-VACNT) were directly grown on copper current collectors via plasma-enhanced chemical vapor deposition (PECVD), forming a binder-free anode structure. This architecture provided improved electrical conductivity, mechanical robustness, and a high specific surface area, which collectively facilitated uniform lithium nucleation and suppressed dendrite formation. The degree and type of nitrogen doping were systematically tuned by varying the nitrogen gas flow rate and RF plasma power. Raman spectroscopy was employed to assess the structural disorder induced by nitrogen incorporation, while X-ray photoelectron spectroscopy (XPS) was utilized to determine the chemical configurations of nitrogen species. Under optimized conditions (300 W RF power, 280 sccm nitrogen flow), a higher D/G intensity ratio and an increased proportion of pyridinic nitrogen were achieved, which correlated with enhanced electrochemical properties. Electrodes fabricated by lithium infusion into the N-VACNT framework demonstrated stable cycling performance exceeding 250 hours in symmetric cell configurations, with low voltage hysteresis. Furthermore, Li–S full cells incorporating these lithium-infused N-VACNT anodes and carbon–sulfur composite cathodes delivered excellent rate capability and capacity retention (~500 mAh g^{-1} at 5C), significantly outperforming cells employing conventional lithium metal anodes. These findings demonstrate that precise control over nitrogen defect chemistry plays a key role in optimizing the structural integrity and electrochemical functionality of VACNT, offering a practical design strategy for stable and dendrite-free anodes in high-performance Li–S battery systems.

Poster 25-019

Carbon-Based Triple-Structured Multifunctional Electrode Design for Polysulfide Trapping in Lithium-Sulfur Batteries

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Lithium–sulfur (Li–S) batteries are considered one of the most promising next-generation energy storage systems due to their high theoretical capacity (~1672 mAh g^{-1}) and energy density (~2600 Wh kg^{-1}), which are significantly higher than those of conventional lithium-ion batteries, as well as the abundance and cost-effectiveness of sulfur. However, the insulating property of sulfur leads to a slow redox reaction. In addition, the dissolution and shuttling of lithium polysulfides (LiPS) during cycling also lead to severe shuttle effects. These barriers result in severe capacity fading and poor cycle stability, ultimately hindering the commercialization of Li–S batteries.

In this study, a carbon-based triple-function freestanding cathode was designed to solve these problems by simple vacuum-filtration. Activated carbon (YP) was employed as the sulfur host to suppress physical dissolution using micropores, while carbon materials with catalysts were introduced to immobilize LiPS through chemical interactions. Additionally, a hybrid conductive network comprising graphene and single-walled carbon nanotubes (SWCNTs) was incorporated to enhance electronic conductivity and facilitate redox kinetics. This integrated structural design simultaneously enables physical confinement, chemical adsorption, and electron transport pathways for effective regulation of polysulfides, thereby improving sulfur utilization.

The proposed multifunctional electrode design presents a rational and integrated approach that simultaneously addresses the main challenges, including the shuttle effect and limited conductivity, by incorporating physical confinement, chemical adsorption, and a conductive carbon framework. This strategy contributes to enhancing electrochemical stability and capacity retention, while also providing a broadly applicable design framework for the development of advanced sulfur cathodes with improved cycling performance and practical feasibility.

Poster 25-020

Application of SnS_2-Based Catalytic Hosts for Enhanced Lithium–Sulfur Batteries

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Lithium–sulfur (Li–S) batteries are considered one of the most promising candidates for next-generation energy storage systems due to their high theoretical energy density and the abundance of sulfur. However, their practical deployment is still hampered by severe challenges, such as the dissolution and shuttle of lithium polysulfides (LiPSs) and sluggish redox kinetics.

In this study, we propose nanoflower-structured tin disulfide (SnS_2) as a cathodic catalyst, rather than an active material, to address these issues. SnS_2 was synthesized via hydrothermal reaction followed by ball milling and heat treatment, and then composited with multi-walled carbon nanotubes (MWCNTs) to form an electrically conductive and mechanically robust framework.

The polar surface of SnS_2 interacts strongly with LiPSs through Lewis acid–base interactions, effectively suppressing their dissolution into the electrolyte. Moreover, the nanoflower morphology offers a high surface area and abundant exposed edges that provide catalytic sites for the redox conversion of sulfur species, thus enhancing the utilization and reversibility of sulfur. The catalytic effect is further attributed to the intrinsic redox-active nature of Sn-based metal sulfides, which facilitate polysulfide conversion reactions.

Current efforts focus on optimizing synthesis parameters such as reaction temperature and duration to control structural and functional characteristics. Comparative evaluations suggest improved polysulfide confinement and redox kinetics compared to conventional S/MWCNT hosts. In future work, heteroatom doping of SnS_2, integration of hybrid catalytic systems, and acid treatment of MWCNTs for surface functionalization will be pursued to further enhance catalytic performance and gain deeper mechanistic insights.

Poster 25-021

A comprehensive study of the role of Metal halide in Na_3SbS_4 solid electrolyte for Sodium Solid State Batteries

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The Na_3SbS_4 sodium solid electrolyte is a promising candidate for developing safe and high-performance Sodium Solid-State Batteries (SSSBs). Electrochemical stability and electrode/electrolyte interfacial compatibility remain major bottlenecks for solid-state batteries. Despite the use of various approaches to address these issues, a highly effective solution remains necessary for SSBs. Herein, we introduce Metal halide as a dopant for the Na_3SbS_4 solid electrolyte, which can simultaneously enhance Sodium ion conductivity and suppress the side reaction between the electrode and electrolyte. A series of Metal halide-doped Na_3SbS_4 was synthesized by a high-energy ball milling method, and the doped electrolyte provided an excellent Na-ion conductivity of ~ 1 mS cm^{-1} at 30°C. Especially, XRD results confirm successful Metal halide doping, which contributes to lattice expansion and improves Na-ion conductivity of the electrolyte. Moreover, the Sodium plating/stripping study shows that Metal halide doped Na_3SbS_4 provides improved interfacial compatibility with the alloy anode. Consequently, the assembled Alloy anode//MH-Na_3SbS_4//NNMFO solid state battery retained a high discharge capacity of ~ 90 mAh g^{-1} at a 0.1 C rate and exhibited superior capacity retention compared to the Pristine Solid state battery. The Metal Halide doping approach presents a promising strategy to achieve high sodium-ion conductivity and electrode/electrolyte interface stability for high-performance Sodium Solid-state Batteries.

Poster 25-022

Engineering High Ionic Conductivity Na_3PS_4 Solid Electrolytes through W and O Co-Doping for Sodium Solid State Batteries

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Na_3PS_4 solid electrolyte is considered a promising candidate for sodium solid-state batteries. However, its low ionic conductivity remains a significant challenge for implementation in high-power battery applications. In this work, we enhance the ionic conductivity of Na3PS4 through the simultaneous substitution of W and O at the P and S sites, respectively. This composition is prepared via a high-energy ball milling process followed by low-temperature heat treatment. The prepared sample is examined through various analysis such as XRD, Raman, FE-SEM, and XPS. Initially, Na_3PS_4 is heat treated at different temperatures (200- 400 ºC), among this achieving a high ionic conductivity of 0.2 mS cm^{-1} at 300 °C. Subsequently, WO3 is substituted into the Na3PS4 solid electrolyte, resulting in a high ionic conductivity of 0.96 mS cm^{-1} for the $Na_{2.9}P_{0.9}W_{0.1}S_{3.7}O_{0.3}$ compositions, which is approximately a 5-fold increase over the pristine Na3PS4 electrolyte. A symmetric cell is fabricated using the prepared solid electrolytes; it shows that WO_3 substitution reduces the polarization at a current density of 0.1 mA cm^{-2}, due to higher ionic conductivity. The sodium solid-state battery is assembled using a solid electrolyte, $NaFe_{1/3}Mn_{1/3}Ni_{1/3}$ cathode, and a $Na_{15}Sn_4$ anode, in which the optimized solid electrolyte delivers a high initial discharge capacity of 118 mAh g^{-1} with a CE of 86.7 %, compared to bare electrolyte (107 mAh g-1 and 82.3 %).

Poster 25-023

Single-Atom Fe Anchored on Graphitic Carbon Nitride for accelerated Redox Kinetics in Lithium-Sulfur Batteires

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Lithium–sulfur (Li–S) batteries are considered one of the most promising candidates for next-generation energy storage due to their high theoretical energy density. However, practical applications are limited by challenges such as the polysulfide shuttle effect, sluggish redox kinetics under lean electrolyte conditions. In this study, we introduce a single-atom iron catalyst embedded in graphitic carbon nitride (Fe SAC@g-C_3N_4) for high-performance lithium sulfur batteries. The g-C_3N_4 with its abundant nitrogen functional groups provides coordination sites for atomically dispersed Fe, effectively stabilizing the metal centers and preventing aggregation. These Fe SAC@g-C3N4 structures also offer strong chemical affinity toward lithium polysulfides, enhancing their immobilization and promoting fast redox conversion. As a result, the Fe SAC@g-C_3N_4 modified separator delivers a high initial discharge capacity of 608 mAh g^{-1} at 0.5C under a high sulfur loading of 3.2 mg cm^{-2} and a lean electrolyte condition of 6 μL mg^{-1}. Moreover, it exhibits excellent long-term cycling stability, retaining 86.2% of its capacity after 400 cycles at 2C. This work demonstrates the synergistic effect of atomic Fe sites and graphitic carbon nitride in enabling high-performance Li–S batteries under practical operating conditions.

Poster 25-024

Lithium Salt-Modified PVDF Binder for Enhanced Lithium– Sulfur Battery Performance

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The practical realization of high-energy-density lithium–sulfur (Li–S) batteries is often limited by poor sulfur utilization under lean electrolyte conditions, particularly in thick electrodes with high sulfur loading. These electrodes typically suffer from low wettability and severe ion/electron transport limitations due to their tortuous structure. In this work, we report a novel binder engineering strategy that modulates the phase of conventional polyvinylidene difluoride (PVDF) using lithium salt-based additives (LiF, LiOH, $LiNO_3$, and LiTFSI). These additives are incorporated into the cathode formulation to enhance the physicochemical properties of thick sulfur electrodes. The modified PVDF exhibits an increased α-phase content, improved surface smoothness, and enhanced electrolyte wettability, which collectively promote better ion transport and sulfur redox kinetics. Among the tested additives, the LiF-modified cathode demonstrates the highest sulfur reactivity of 56.4%, delivering a specific capacity of 945 mAh g^{-1} at an electrolyte-to-sulfur (E/S) ratio of 8 μL mg^{-1}. This corresponds to a 35% increase in the amount of reactive sulfur compared to the pristine PVDF-based electrode. Furthermore, a Li–S pouch cell with a 200 μm-thick cathode and 4.0 mg cm^{-2} sulfur loading is successfully operated under lean electrolyte conditions, highlighting the scalability and practicality of this approach. This study offers a promising pathway toward the development of ultrathick, high- loading sulfur cathodes compatible with low-electrolyte Li–S battery systems.

Poster 25-025

Separator Coating Strategy for Room-Temperature Na–S Batteries Using Ether-Based Electrolytes

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Sodium-Sulfur (Na–S) batteries are emerging as attractive candidates for next-generation energy storage due to their high theoretical energy density, cost-effectiveness, and the widespread availability of sodium. Nevertheless, their practical viability remains limited by the pronounced shuttle effect of soluble polysulfides, particularly in ether-based electrolytes, which undermines capacity retention and cycling performance.

While ester-based electrolytes mitigate polysulfide solubility, they often operate at lower voltages and necessitate costly additives such as fluoroethylene carbonate (FEC). Ether-based systems, on the other hand, offer higher voltage windows and additive-free operation, but they are prone to severe polysulfide diffusion.

To overcome these limitations, we designed a functional separator with a composite coating of vanadium nitride-doped reduced graphene oxide (rGO@VN). This coating acts as both a polysulfide-adsorbing layer thanks to its polar characteristics and as a redox catalyst that accelerates the conversion of intermediate species, thereby enhancing reaction kinetics. Comprehensive electrochemical characterization, including in situ Raman spectroscopy and electrochemical impedance spectroscopy (EIS), revealed that the rGO@VN-modified separator effectively reduces polysulfide accumulation and promotes their sequential transformation during cycling.

Our findings highlight a promising separator modification strategy for ether-based Na–S batteries, offering improved cycle life and capacity without relying on expensive electrolyte additives.

Poster 25-026

Suppressing Lithium Dendrite Penetration via Lithiophilic Interlayers in Garnet Solid Electrolytes

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All-solid-state batteries (ASSBs) have emerged as a promising technology for next-generation energy storage, providing enhanced safety through non-flammable solid electrolytes and high energy density with lithium-metal anodes[1]. Among solid electrolytes, the garnet-type solid electrolyte $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ (LLZTO) has attracted significant attention due to its high ionic conductivity and excellent chemical stability against lithium metal[2-4]. However, uncontrolled lithium dendrite penetration through the solid electrolyte remains a critical bottleneck, often causing short-circuit failure even at low current densities[5]. This problem stems from interfacial inhomogeneity driven by poor lithium wettability at the Li metal/LLZTO interface. Although various lithiophilic interlayers have explores, existing approaches have not yet achieved sufficient performance for practical applications[6-13].

Here we report a facile drop-coating method using metal chlorides to form a uniform lithiophilic interlayer at the Li metal/LLZTO interface. This approach significantly reduces interfacial resistance and enables uniform lithium plating and stripping, thereby markedly increasing the critical current density. Furthermore, long-term galvanostatic cycling demonstrates excellent electrochemical stability, highlighting the potential of this approach for practical ASSB operation. These findings provide key insights into interfacial engineering and establish a viable route toward the commercialization of garnet-based all-solid-state battery systems.

References

[1] Q. Zhao, S. Stalin, C. Z. Zhao, L. A. Archer, Nat. Rev. Mater., **5**, (2020) 229-252.

[2] L. J. Miara, S. P. Ong, Y. Mo, W. D. Richards, Y. Park, J. M. Lee, H. S. Lee, G. Ceder, *Chem. Mater.*, **25**, (2013) 3048-3055.

[4] F. Han, A. S. Westover, J. Yue, X. Fan, F. Wang, M. Chi, D. N. Leonard, N. J. Dudney, H. Wang, C. Wang, Nat. Energy, **4**, (2019) 187-196.

[5] A. Sharafi, H. M. Meyer, J. Nanda, J. Wolfenstine, J. Sakamoto, *J. Power Sources*, **302**, (2016) 135-139.

[6] H. Huo, Y. Chen, N. Zhao, X. Lin, J. Luo, X. Yang, Y. Liu, X. Guo, X. Sun, *Nano Energy*, **61**, (2019) 119-125.

[7] T. Krauskopf, F. H. Richter, W. G. Zeier, J. Janek, Chem. Rev., **120**, (2020) 7745-7794.

[8] R. Murugan, V. Thangadurai, W. Weppner, Angew. Chem. Int. Ed., **46**, (2007) 7778-7781.

[9] B. Liu, L. Zhang, H. Xu, L. McEntush, G. Fang, M. S. Wang, L. Xie, B. Xu, L. Lu, J. Liang, C. Wang, Nat. Commun., **11**, (2020) 2278.

[10] Y. Zhong, Y. Xie, S. Hwang, Q. Wang, J. J. Cha, D. Su, H. Wang, A, *Angew. Chem. Int. Ed*., **59**, (2020) 14003-14008.

[11] W. Luo, Y. Gong, Y. Zhu, Y. Li, Y. Yao, Y. Zhang, K. Fu, G. Pastel, C.-F. Lin, Y. Mo, E. D. Wachsman, L. Hu, *Adv. Mater*., **29**, (2017) 1606042.

[12] J. Meng, Y. Zhang, X. Zhou, M. Lei, C. Li, *Nat. Commun*., **11**, (2020) 3716.

[13] Y. Zhang, J. Meng, K. Chen, H. Wu, J. Hu, C. Li, *ACS Energy Lett*., **5**, (2020) 1167-1176.

Poster 25-027

Fabrication of $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ Solid Electrolytes by Tape Casting for All-Solid-State Batteries

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Lithium metal batteries (LMBs) are considered the pinnacle of electrochemical energy storage, offering an unprecedented theoretical capacity of 3,860 $mAh \cdot g^{-1}$) through the use of metallic lithium anodes [1]. However, uncontrolled dendrite growth during cycling induces short-circuit failure [2]. When coupled with conventional liquid electrolytes, such failures can trigger thermal runaway with severe safety consequence [3]. All-solid-state batteries (ASSBs), employing non-flammable solid electrolytes, offer a transformative pathway to overcome these limitations [4].

Among candidate electrolytes including polymers, sulfides, and oxides, oxide-based systems combine mechanical strength, electrochemical stability, and chemical inertness [5,6]. In particular, garnet-type $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$ (LLZTO) has garnered particular attention owing to its high ionic conductivity ($\sim 10^{-3}$ $S \cdot cm^{-1}$) and stability against lithium reduction [7,8].

However, to achieve commercial viability, oxide electrolytes need to fabricated in ~20 μm thickness comparable polymer separators in lithium-ion batteries [9]. While wet-chemical deposition can produce such thin films, scalability and cost remain prohibitive. In contrast, tape-casting offers a low-cost, industrially relevant pathway for large-scale manufacturing [10].

Here, we report the scalable fabrication of ultra-thin LLZTO electrolyte sheets via an optimized tape-casting methodology. Using commercial LLZTO powders, tailored slurries are formulated and processed by doctor-blade casting to produce thin green tapes. Post-sintering characterization demonstrates dense microstructures and single-phase cubic garnet crystallinity via X-ray diffraction analysis. Electrochemical impedance spectroscopy showed a high ionic conductivity of 5.31×10^{-4} $S \cdot cm^{-1}$, validating the electrochemical integrity of these thin electrolytes. This scalable approach addresses critical thickness constraints as a viable platform for next-generation Li-based all-solid-state batteries.

Keywords: All solid-state battery, LLZTO, garnet structure, tape casting method.

References

[1] A. Manthiram, X. Yu, S. Wang, Nat. Rev. Mater. **2** (2017) 16103.

[2] Huang, Y., Yang, H., Gao, Y., Chen, G., Li, Y., Shi, L., & Zhang, D. (Year). Title of the article. Journal Name, *Mater. Chem. Front.,* (2024), **8**, 1282-1299

[3] Y. Guo, H. Li, T. Zhai, *Adv. Mater*. **29** (2017) 29.

[4] J. Janek, W. G. Zeier, *Nat. Energy*. **1** (2016) 16141.

[5] L. J. Miara, S. P. Ong, Y. Mo, W. D. Richards, Y. Park, J. M. Lee, H. S. Lee, G. Ceder, *Chem. Mater*. **25** (2013) 3048-3055.

[6] K. V. Kravchyk, D. Tarik Karabay, M. V. Kovalenko, *Sci. Rep.* **12** (2022) 1177.

[7] Murugan R., Thangadurai V., Weppner W., *Angew. Chem. Int. Ed.* **46** (2007) 7778-7781.

[8] Y. Zhu, X. He, Y. Mo, ACS Appl. *Mater. Interfaces* **7** (2015) 23685-23693.

[9] L. Li, Y. Dian, *Polymers*, **15**, (2023) 3690.

[10] Parascos K., Watts J. L., Alarco J. A., Talbot P. C., *J. Energy Storage* **92** (2024) 111996.

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Electrochemical Characterization of LICs with Ni-rich Cathodes and Direct Contact Pre-lithiated Anodes

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With the continuous increase in the demand for electric vehicles and electric trucks, batteries are expected to meet the requirements of high energy density, high power capability, and long cycle life.

Lithium-ion Batteries, using lithium metal oxides as cathodes and graphite as the main anode material, provide high energy density. In contrast, Lithium-ion Capacitors provide power capability and long cycle life, but pre-lithiation of the anode is required to reduce the intial irreversible capacity loss. Several pre-lithiation techniques have been studied, including electrochemical, direct contact, and wet chemical methods, with growing emphasis on process simplification. Among them, the electrochemical approach consists of two methods: one method performs pre-lithiation externally using a half cell before applying it to a full cell, and the other introduces a lithium source inside the full cell to conduct electrochemical pre-lithiation after assembly. When electrochemical pre-lithiation is carried out outside the cell, it has the advantage of precisely controlling the amount of lithium insertion. However, it also has the disadvantages of being time-consuming and making the process more complex. In contrast, the method using an internal lithium source after cell assembly has the advantages of a simple process and immediate applicability, but it is difficult to uniformly control the lithium insertion. The direct contact method, in which lithium foil is placed in direct contact with the anode, makes the control of variables manageable but has the limitation of requiring a long processing time.

In this study, a new method is proposed that combines direct contact pre-lithiated anodes with an internal electrochemical approach using Ni-rich cathode materials, in order to reduce the time required for the contact process. The direct contact pre-lithiation was carried out by adjusting the contact duration and the compression load between the lithium foil and the anode, and the deficiency of lithium was supplemented by regulating the NCM content in the cathode. This approach is expected to simplify the pre-lithiation process for LICs, while making the control of variables more manageable and at the same time fulfilling the requirements of high energy density, high power capability, and long cycle life.