

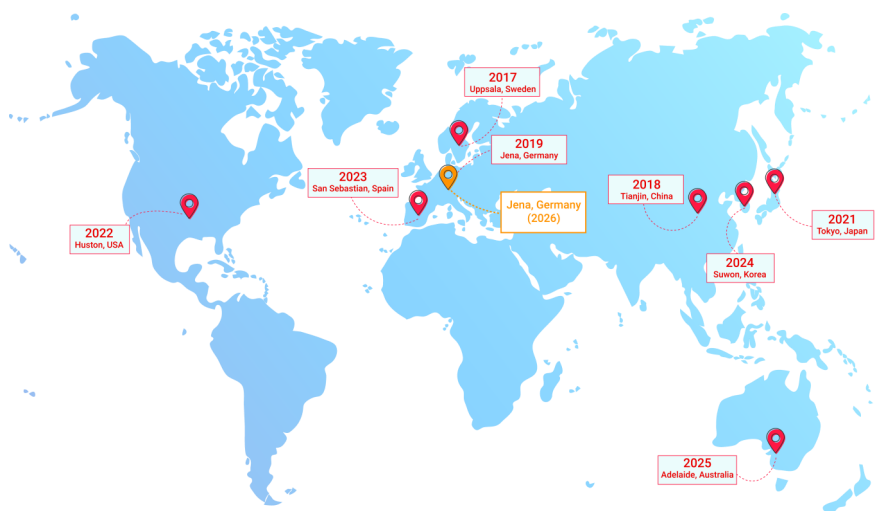


ORGANIC BATTERY DAYS 2026

Conference Book

5–7 October 2026 | Jena (Germany)

HISTORY OF ORGANIC BATTERY DAYS



CONFERENCE BUILDING



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GENERAL INFORMATION

Date

5–7 October 2026

Venue

Friedrich Schiller University Jena
CEEC Jena II / AWZ CEEC Jena
Lessingstraße 12–14
07743 Jena
Germany

Please note that the capacity of the lecture hall is strictly limited!
Live video transmissions to other rooms will be made available.

Scientific Advisory Board

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WELCOME NOTE

Dear friends and colleagues,

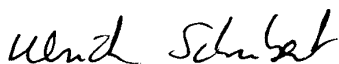
It is my great pleasure to welcome you to Organic Battery Days 2026 in Jena.

This international three-day conference brings together experts from science, research, politics, administration, and industry to exchange knowledge and experience on the latest developments in the field of electrochemical energy storage based on organic active materials. The conference offers an excellent opportunity for scientific exchange, inspiring discussions, and new collaborations within the growing field of organic batteries.

Over the course of the conference, participants can look forward to a diverse scientific programme including invited lectures, oral contributions, poster presentations, and opportunities for networking and personal exchange.

I am delighted to welcome you to Jena and wish you a stimulating conference, fruitful discussions, and a pleasant stay.

Sincerely yours,

A handwritten signature in black ink, reading 'Ulrich Schubert' in a cursive script.

Prof. Dr. Ulrich S. Schubert



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Password:

Dhmo9bgen

SCIENTIFIC PROGRAMME

Monday, 5 October 2026

PL Plenary lecture
IL Invited lecture
CL Contributed lecture

08:00–08:45 REGISTRATION

08:45–09:10 CONFERENCE OPENING & WELCOME

Prof. Dr. Ulrich S. Schubert

Chairman

Friedrich Schiller University Jena, Germany

Prof. Dr. Andreas Marx

*President of the Friedrich Schiller University Jena,
Germany*

09:10–09:50 SESSION 1: Battery Systems & Cell Concepts

PL| Prof. Dr. Jodie Lutkenhaus

Texas A&M College of Engineering, USA

Organic batteries for low temperature operation

09:50–10:20 **IL| Prof. Dr. Xinliang Feng**

TUD Dresden University of Technology, Germany

Aqueous metal-ion batteries - from printable
electronics to large-scale energy storage systems

10:20–10:50 **Coffee break**

10:50–11:20 SESSION 2: Mechanisms & Advanced Characterization

IL| Prof. Dr. Michael J. Aziz

*Harvard University John A. Paulson School of Engineering
and Applied Sciences, USA*

Molecular lifetime, capacity fade and capacity recovery
with organic active species

11:20–11:50 **IL| Prof. Dr. Hirofumi Yoshikawa**

Kwansei Gakuin University, Japan

Multi-valent ion batteries using organic framework
structure materials

11:50–12:20 **IL| Prof. Dr. Steven Renault**

French National Centre for Scientific Research, France

Unlocking the second electron in the electrochemical
delithiation-lithiation of p-DHT derivatives - Cu²⁺ effect

SCIENTIFIC PROGRAMME

- 12:20–12:50 **IL| Dr. Ingo Manke**
Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
Three-dimensional morphology of polymer-based batteries - combining tomographic 3D imaging with modeling and simulation
- 12:50–13:10 **Conference photo**
- 13:10–14:10 **Lunch**
- SESSION 3: Battery Systems & Cell Concepts**
- 14:10–14:40 **IL| Dr. Nerea Casado**
POLYMAT, Spain
Molecular design of high-potential PROXYL radicals for advanced organic batteries
- 14:40–15:10 **IL| Prof. Dr. Nara Kim**
Linköping University, Sweden
Sustainable stretchable organic batteries for wearable electronics
- 15:10–15:30 **CL| Dr. Nagaraj Patil**
IMDEA Energy Institute, Spain
From redox polymers to practical electrodes: engineering high areal capacity in organic batteries
- SESSION 4: Materials Design & Synthesis**
- 15:30–15:50 **CL| Prof. Dr. Jiande Wang**
College of Materials Science and Engineering, Hunan University, China
Conjugated sulfonamides for next generation energy storage
- 15:50–16:10 **CL| Prof. Dr. Ji Eon Kwon**
Korea Institute of Science and Technology, Republic of Korea
Indolocarbazole: a high-voltage multi-electron p-type redox center for organic electrode materials

SCIENTIFIC PROGRAMME

- 16:10–16:30** **CL| Dr. Ryota Akai**
National Institute of Advanced Industrial Science and Technology (AIST), Japan
Redox-active porous organic cage as a positive-electrode material for rechargeable lithium batteries
- 16:30–17:00** **Coffee break**
- 17:00–17:20** **CL| Prof. Dr. Philippe Poizot**
Nantes Université/CNRS-IMN, France
Electrochemical evaluation of extended viologens as negative electrode materials for anion-ion rechargeable batteries
- 17:20–17:40** **CL| Prof. Dr. Edwin Otten**
University of Groningen, Netherlands
Molecular insights into capacity fade in non-aqueous redox flow batteries
- 17:40–18:00** **CL| Prof. Dr. Riccardo Alessandri**
KU Leuven, Belgium
Multiscale modeling of structural, ionic, and electronic properties of radical-containing polymers for all organic Batteries
- 18:00–18:20** **CL| Prof. Dr. Doreen Mollenhauer**
Helmholtz Institute for Polymers in Energy Applications Jena, Germany
Computational exploration of structure-property relationships in redox-active organic materials
- 18:20–18:40** **CL| Dr. Daniel Tabor**
Department of Chemistry, Texas A&M University, USA
First-principles and machine learning strategies for modeling organic batteries

SCIENTIFIC PROGRAMME

18:40–19:00 **CL| Dr. Clara Zens**
Friedrich Schiller University Jena, Germany
Molecular insights into charge transport in conjugated radical batteries

EVENING EVENTS

19:00 **Walk to Botanical Garden**

19:30 **Welcome and Opening at Botanical Garden (speakers, registered participants with regular fee)**

and

19:15 **PhD and Early-stage Researcher Networking & Discussions (drinks / snacks)**
Conference site

SCIENTIFIC PROGRAMME

Tuesday, 6 October 2026

08:00–08:30 **REGISTRATION**

08:30–09:10 **SESSION 7: Battery Systems & Cell Concepts**

PL| Prof. Dr. Birgit Esser

Ulm University, Germany

Organic electrode materials in next-generation batteries

09:10–09:40 **IL| Dr. Rebeca Marcilla**

IMDEA Energy Institute, Spain

Membrane-free redox flow batteries - design strategies and performance enhancement

09:40–10:00 **CL| Prof. Dr. Zhongfan Jia**

Flinders University, Australia

Caging polyhalide anions in polycyclodextrin for long-lasting aqueous zinc-iodine batteries

10:00–10:20 **CL| Dr. Carlo Caianiello**

Division of Organic Chemistry, Department of Chemistry, KTH Royal Institute of Technology, Sweden

Bipolar molecules and posolytes for aqueous organic flow batteries: exploring new chemistries for different pH

10:20–11:00 **Coffee break**

11:00–11:30 **SESSION 8: Sustainability, Circularity & Translation**

IL| Dr. Cedrik Wiberg

Rivus Batteries GmbH, Germany

Challenges and experiences from commercializing organic flow batteries

11:30–12:00 **IL| Dr. Tobias Janoschka**

Jena Flow Batteries GmbH, Germany

From milliwatts to megawatts - bringing an organic flow battery technology to scale

SCIENTIFIC PROGRAMME

- 12:00–12:20** **CL| Prof. Dr. Klaus Meerholz**
University of Cologne, Germany
How “green” is your functional material? Assessing environmental impacts of multi-step synthetic protocols in material sciences at various technology levels
- 12:20–12:40** **CL| Kristína Rabatinová**
Friedrich Schiller University Jena, Germany
Life-cycle assessment of organic redox flow batteries for long-duration energy storage
- 12:40–13:00** **CL| Dr. Tilmann J. Neubert**
Friedrich Schiller University Jena, Germany
Sustainable quinones at electrochemical interfaces: what can we learn from organic batteries for adhesives and carbon capture?
- 13:00–14:00** **Lunch**
- 14:00–15:30** **Parallel breakout sessions**
1) Battery characterization at Helmholtz Zentrum Berlin: BESSY II and tomography
Prof. Dr. Yan Lu, Dr. Ingo Manke, Anna Anochin
2) DFG Priority programme “Polymer-based Batteries” (SPP 2248): selected topics
3) Laboratory Tours: HIPOLE Jena and FSU Jena
4) From modeling to advanced physicochemical characterization of polymers: understanding organic battery materials at HIPOLE Jena/CEEC
Prof. Dr. Doreen Mollenhauer, Prof. Dr. Ivo Nischang
- 15:30–16:00** **Coffee break**

SCIENTIFIC PROGRAMME

SESSION 9: Materials Design & Synthesis

16:00–16:20

CL| Prof. Dr. Matthieu Becuwe

LRCS UPJV-CNRS, France

Conductive positive electrode materials using molecular and material engineering

16:20–16:40

CL| Dr. Lionel Dubois

Commissariat à l'énergie atomique (CEA), France

A systematic study of hydroquinone dicarboxylate isomers for Li-ion batteries applications

16:40–17:00

CL| Dr. Rukiya Matsidik

TU Chemnitz, Germany

Aromatic diimides: versatile building blocks for organic battery electrode materials

SESSION 10: Mechanisms & Advanced Characterization

17:00–17:20

CL| Emilio Avellone

Technical University of Munich (TUM), Germany

Massachusetts Institute of Technology (MIT), USA

Diagnosing performance-limiting factors in iron–AQDS redox flow batteries

17:20–17:40

CL| Dr. Koosha Ehtiati

Friedrich Schiller University Jena, Germany

Electrochemical characterization of flow battery active materials: rotating disc electrode voltammetry vs. electrochemical impedance spectroscopy

17:40–18:00

CL| Jonathan Caroni

CiQus, Universidade de Santiago de Compostela, Spain

Advanced organic polymer electrodes for lithium and sodium-ion batteries

SCIENTIFIC PROGRAMME

POSTER SESSION

18:00–21:00

Poster session (drinks/snacks)

Session 1: 18:00–19:30

Session 2: 19:30–21:00

Dinner buffet start: 19:00

ZAF Atrium (Center for Applied Research)

19:00–20:00

Scientific advisory board meeting

(internal meeting)

ZAF SpaceBox 10G

SCIENTIFIC PROGRAMME

Wednesday, 7 October 2026

08:00–08:30 **REGISTRATION**

- 08:30–09:10 **SESSION 11: Electrolytes, Interfaces & Transport**
PLJ Prof. Dr. Ho Seok Park
Sungkyunkwan University (SKKU), Republic of Korea
Two-dimensional organic frameworks for electrolyte and interfacial engineering in lithium metal batteries
- 09:10–09:40 **ILJ Prof. Dr. Jean-François Gohy**
Université catholique de Louvain, Belgium
Novel approaches towards polymer-based electrolytes
- 09:40–10:00 **CLJ Prof. Dr. Kenichi Oyaizu**
Waseda University, Japan
Polymers to stabilize the supercooled liquid state of Li salts: An approach to organic solid-state batteries
- 10:00–10:20 **CLJ Prof. Dr. Andrea Balducci**
Friedrich Schiller University Jena, Germany
The impact of electrolyte formulation on the electrochemical performance of PTMA-based electrodes
- 10:20–11:00 **Coffee break**
- 11:00–11:20 **SESSION 12: Mechanisms & Advanced Characterization**
CLJ Prof. Dr. Shrayesh Patel
University of Chicago, USA
Mediator-driven redox targeting for polymeric flow batteries
- 11:20–11:40 **CLJ Dr. Leslie Rocio Arias-Aranda**
Institut des Sciences Chimiques de Rennes, Université de Rennes, France
Symmetric aqueous redox flow batteries and reference ferri/ferrocyanide pair: A critical look on the stability of ferrocene derivatives at neutral pH

SCIENTIFIC PROGRAMME

- 11:40–12:00 **CL| Dr. Michael Walter**
University of Freiburg / FIT, Germany
Characterizing sulfur–organic networks formed by
inverse vulcanization using X-ray spectroscopy
- 12:00–12:20 **CL| Dr. Klemen Pirnat**
National Institute of Chemistry, Slovenia
Study of four-electron exchange on benzene and naphthalene ring
- SESSION 13: Materials Design & Synthesis
- 12:20–12:40 **CL| Dr. Tianyang Chen**
The Chinese University of Hong Kong (Shenzhen), China
Sustainable 2D layered cathode for alkali-ion batteries
- 12:40–13:00 **CL| Julie Schulz**
LRCS UMR 7314, France
Synthesis of organic macromolecular materials for solid organic batteries
- 13:00–13:20 **CL| Rika Yamamoto**
Keio University, Japan
Exploration of quinone-based polymers for organic cathode active materials of lithium-ion batteries
- 13:20–13:40 **CONCLUDING REMARKS**
Poster Prizes
Concluding Remarks & Farewell
Prof. Dr. Ulrich S. Schubert
- 13:40 **Light lunch**

Abstracts of Plenary Speakers

ABSTRACTS OF PLENARY SPEAKERS

Organic batteries for low temperature operation

Prof. Dr. Jodie Lutkenhaus

Texas A&M College of Engineering

Lithium-ion batteries have been widely used in portable electronic devices for many years. However, these batteries still face significant challenges in harsher and more complex environments such as electric vehicles, aerospace, subsea operations, and power grid systems. Specifically, lithium-ion batteries lose their ability to charge and discharge at low temperatures due to freezing of the electrolyte, as well as impeded desolvation of ions at the electrode-electrolyte interface. This talk will focus on redox-active polymers as potential active materials for low-temperature batteries. In the first portion of the talk, a dual-ion battery comprised of copolymer of 2,2,6,6-tetramethyl-piperidinyloxy-4-yl methacrylate and glycidyl methacrylate (PTMA-co-GMA) and naphthalene tetracarboxylic dianhydride-derived polyimide (PNTCDI) as active materials for the positive and negative electrodes, respectively, is discussed. Using a low-temperature electrolyte, the dual-ion battery exhibited a capacity of 76 mAh g at 1C current, maintaining operability up to 10C current, and delivering 1000 W kg specific power down to -40 °C. The battery maintained 85% capacity at 0°C and 55% capacity at -40 °C. Interestingly, the battery showed near-zero capacity decay while cycling at low temperatures. The second portion of this talk will present a fundamental investigation of energy barriers associated with low temperature operation in organic batteries, illustrating specific cases in which organic batteries can out-perform lithium-ion batteries. Taken together, organic batteries demonstrate a promising path toward earth-abundant energy storage materials for extreme environments.

ABSTRACTS OF PLENARY SPEAKERS

Organic electrode materials in next-generation batteries

Prof. Dr. Birgit Esser

Ulm University

Organic electrode materials have attracted great interest for next-generation batteries, in particular so-called post-lithium batteries,^[1] including multivalent metal and anionic batteries. They can be classified into p- and n-type organic materials and can therefore furnish different types of battery cell configurations: cation-rocking chair, anion-rocking chair and dual-ion,^[2,3] which include metal- and all-organic batteries. In this talk the design,^[4] synthesis^[5] and operational principles of selected p- and n-type organic electrode materials will be discussed as well as their application in all-organic^[6,7] and “post-lithium”-metal full cells.^[8–10]

References:

- [1] B. Esser, H. Ehrenberg, M. Fichtner, A. Groß, J. Janek, *Adv. Energy Mater.* **2025**, *15*, 2402824.
- [2] R. Wessling, P. Penert, B. Esser, *Adv. Energy Mater.* **2025**, *15*, 2500150.
- [3] B. Esser, F. Dolhem, M. Becuwe, P. Poizot, A. Vlad, D. Brandell, *J. Power Sources* **2021**, *482*, 228814.
- [4] P. Penert, B. Schulz, A. Florent, P. Poizot, B. Esser, *ACS Appl. Polym. Mater.* **2026**, *8*, 5929–5939.
- [5] F. Adler, S. Pinto-Bautista, C. Lorenz, L. Hinrichs, M. Weil, B. Esser, *Adv. Sci.* **2025**, e2506251.
- [6] R. Wessling, H. Koger, F. Otteny, M. Schmidt, A. Semmelmaier, B. Esser, *ACS Appl. Polym. Mater.* **2024**, *6*, 7956–7968.
- [7] P. Penert, L. S. Neige, C. Lorenz, W. Stawski, B. Esser, *Adv. Energy Sustain. Res.* **2026**, *7*, e202500496.
- [8] G. Studer, A. Schmidt, J. Büttner, M. Schmidt, A. Fischer, I. Krossing, B. Esser, *Energy Environ. Sci.* **2023**, *16*, 3760–3769.
- [9] S. M. Pallasch, M. Bhosale, G. J. Smales, C. Schmidt, S. Riedel, Z. Zhao-Karger, B. Esser, O. Dumele, *J. Am. Chem. Soc.* **2024**, *146*, 17318–17324.
- [10] M. Adil, R. Wessling, N. Kokott, E. Mena-Osteritz, B. Prifling, M. Osenberg, T. Diemant, V. Schmidt, I. Manke, B. Esser, *Adv. Energy Mater.* **2026**, 71098.

ABSTRACTS OF PLENARY SPEAKERS

Two-dimensional organic frameworks for electrolyte and interfacial engineering in lithium metal batteries

Prof. Dr. Ho Seok Park

Sungkyunkwan University (SKKU)

The practical realization of lithium metal batteries is fundamentally constrained by uncontrolled dendrite growth, parasitic side reactions, and mechanically fragile solid electrolyte interphases — all rooted in poorly regulated ion transport and interfacial chemistry. Two-dimensional (2D) organic-based materials, owing to their structural programmability and tunable functional sites, offer a compelling platform to simultaneously address these challenges across both liquid and solid electrolyte systems.

In the first strategy, I will introduce molecularly engineered 2D polymeric metal phthalocyanines (CoTP) conformally coated on carbon surface, which can direct localised TFSI⁻ anion flux toward the electrode surface for uniform LiF-rich SEI formation, as well as facilitate interfacial Li⁺ transfer through pseudo-crown ether-type TEG linkers. Then, I will address 2D dual-Lewis-base covalent organic framework (N/O-COF) bearing triazine and carbonyl groups integrated into PEO-based solid polymer electrolytes. The synergistic N/O coordination environment simultaneously enables directional Li⁺ migration through ordered nanochannels and promotes LiF-rich SEI formation via TFSI⁻ decomposition. Together, these works establish 2D organic frameworks as a powerful and generalisable design platform for governing both bulk ionic environments and electrode–electrolyte interfacial chemistry, offering a fundamental pathway toward safe, high-energy, and durable lithium metal batteries.

Abstracts of Invited Speakers

ABSTRACTS OF INVITED SPEAKERS

Novel approaches towards polymer-based electrolytes

Prof. Dr. Jean-François Gohy

Université catholique de Louvain

Compared to conventional liquid electrolytes, polymer-based solid and quasi-solid-state electrolytes (e.g., ionogel) exhibit enhanced safety and broader electrochemical stability windows, enabling compatibility with high-voltage cathodes. While their improved mechanical robustness (compared with liquid electrolyte) is often highlighted, the lithium-ion transport mechanism in these systems—polymer segmental dominated motion—imposes an inherent trade-off between ionic conductivity and mechanical strength. To overcome this compromise, it is necessary to develop an ionic transport mechanism where lithium ions migrate independently of the host polymer chain dynamics. Its realization demands a focus shift in materials design from conventional polymer chains mobility to other environment engineering or transport pathways. Crucially, if such a mechanism becomes the dominant transport mode, it may decouple ion migration from polymer chain dynamics—fundamentally shifting the prevailing paradigm. This would open a pathway toward materials that simultaneously exhibit high ionic conductivity and mechanical strength.

One possibility relies on the so-called competitive coordination principle, creating an environment in which lithium ions are shared between multiple ligands with similar binding energy. In polymer-based ionogels, this can be achieved by combining polymer networks with ionic liquids. Lithium ions in such systems do not form strong coordination with any single ligand, resulting in reduced average binding energies and enhanced ion lability. Although competitive coordination has been widely explored in liquid electrolyte systems, its application in solid and quasi-solid polymer electrolytes remains in its infancy. Herein, we design a crosslinked polyrotaxane network and then introduce ionic liquid and a lithium salt to obtain an ionogel electrolyte based on the principle of competitive coordination with the lowest binding energy for lithium ions coordinated with both the polymer network and ionic liquid clusters. This facilitates their migration within the ionogel and their release from the coordination environment, thereby improving lithium-ion transport efficiency (ionic conductivity of $2.2 \times 10^{-3} \text{ S cm}^{-1}$ and $t_{\text{Li}^+} = 0.45$ at 20°C).¹

Another possibility lies in the use of liquid crystalline block copolymer electrolytes (BCPE) with a liquid crystal and a lithium-ion conductive phase. Herein, we synthesize a lithium salt loaded poly(10-[(4-cyano-4'-biphenyl)oxy] decatyl methacrylate)-block-(methoxy-poly(ethylene glycol) methacrylate-co-glycidyl methacrylate) [P(MALC)-b-P(PEGMA-co-GM)] BCPE by reversible addition-

ABSTRACTS OF INVITED SPEAKERS

fragmentation transfer polymerization. Formation of a smectic A mesophase in a broad temperature range was confirmed for those samples with or without added lithium salt. A setup was developed to drop-cast BCPE solutions into a homogeneous E_F (AC or DC) under controlled conditions. Self-standing films were obtained and employed for further electrochemical and morphological analysis. Samples subjected to E_F consistently exhibited enhanced ionic conductivity, reaching values up to $4.7 \cdot 10^{-5} \text{ S} \cdot \text{cm}^{-1}$ at 60°C , compared to $6.0 \cdot 10^{-6} \text{ S} \cdot \text{cm}^{-1}$ at the same temperature for the polymer electrolyte casted without E_F . Hierarchical morphologies at two nanoscales were identified across a broad range of examined BCPE compositions. In all recognized microstructures, the discrete smectic A layers exhibited a perpendicular orientation with respect to the BCPE. The observed increase in ionic conductivity is attributed to the stronger phase separation and longer-range order achieved through E_F directed self-assembly, that further allow the creation of efficient lithium-ion transport pathways between the different microphases of the BCPE.²

References

- [1] S. Yan, J. Liu, Z. He, H. Jia, Z. Chen, Y. Zhang, J.-F. Gohy, *Angew. Chem. Int. Ed.* **2025**, 64, e202503307.
- [2] I. Álvarez Moisés, M. Król, G. Keus, Z. He, A. Innocenti, S. Passerini, J. Ruokolainen, J.-F. Gohy, *J. Am. Chem. Soc.* **2025**, 147, 20347–20358.

ABSTRACTS OF INVITED SPEAKERS

Multi-valent ion batteries using organic framework structure materials

Prof. Dr. Hirofumi Yoshikawa

Kwansei Gakuin University

Calcium-ion batteries (CIBs) are promising energy storage systems because of their low cost and high theoretical volumetric energy density. However, calcium ion (Ca^{2+}), a divalent cation with a larger ionic radius than lithium ion, forms strong electrostatic interactions with the divalent O^{2-} anion in conventional metal-oxide-based cathode active materials, resulting in capacities less than 55% of the theoretical values and poor rate performance. In this study, $\text{Cu}_3(\text{HHTP})_2$ (HHTP: 2,3,6,7,10,11-hexahydroxytriphenylene), a two-dimensional metal-organic framework with monovalent O^- anions included in its crystal structure, is used as a cathode active material for CIBs, and its performance, as well as its calcination and de-calcination mechanisms, is investigated. $\text{Cu}_3(\text{HHTP})_2$ has a high initial capacity equal to 86% of the theoretical value and excellent rate performance owing to sufficient redox reaction and smooth calcination, respectively. However, it exhibits poor cycle performance because of insufficient de-calcination during charging, which results from electrostatic interactions between intercalated Ca^{2+} ions with O^- anions in the narrower interlayer spacing of $\text{Cu}_3(\text{HHTP})_2$ after the first discharge. These findings provide valuable insights for improving the performance of cathode active materials for CIBs.

References

[1] K. Wakamatsu, S. Ohkata, M. Kajiwara, N. Tanifuji, H. Yoshikawa, T. Shimizu, *ACS Electrochem.* **2026**, 2, 596–603.

ABSTRACTS OF INVITED SPEAKERS

Aqueous metal-ion batteries: From printable electronics to large-scale energy storage systems

Prof. Dr. Xinliang Feng

TU Dresden

Max Planck Institute of Microstructure Physics

Batteries are central to the global decarbonization strategy, enabling the transition from fossil fuels to renewable energy systems. It is projected that the global demand for battery capacity will increase from the current 2–3 TWh to over 9–10 TWh within the next decade, driving rapid expansion of the energy storage market. However, state-of-the-art technologies, including lithium-ion batteries (LIBs), lead–acid batteries (LABs), and nickel–metal hydride batteries (NiMHs), face critical challenges such as limited resource availability (e.g., Li, Co, Ni, and graphite), safety concerns, toxicity, and self-discharge, which hinder their sustainable large-scale deployment. In this context, aqueous metal-ion batteries (AMIBs) have emerged as a promising alternative, offering intrinsic safety, low cost, environmental benignity, and scalability. These systems, encompassing monovalent (Li^+ , Na^+ , K^+), multivalent (Zn^{2+} , Al^{3+}), and proton-based chemistries, hold considerable potential for both grid-level storage and emerging electronics. Nevertheless, their practical implementation remains limited by fundamental challenges, including the narrow electrochemical stability window of water, insufficient cathode capacity, interfacial instability, and dendrite formation at metal anodes. In this talk, I will present our recent advances in addressing these challenges through the design of novel materials and device concepts. In particular, we focus on two-dimensional (2D) organic and inorganic layered materials as highly tunable platforms for electrode active materials, as well as functional interfaces and membranes. Complementary to this, we develop advanced aqueous and quasi-solid-state electrolytes to regulate interfacial reactions and expand the operational window. By integrating these components, we explore diverse cell configurations, including rocking-chair, dual-ion, and flow-type systems, to bridge fundamental materials design with practical device architectures. Furthermore, we extend these concepts toward flexible and printable energy storage devices. By employing printable graphene and 2D materials as functional inks, we demonstrate aqueous and solid-state batteries compatible with scalable fabrication technologies, targeting applications in wearable electronics and distributed energy systems. These efforts highlight a pathway toward next-generation aqueous battery technologies that unify safety, sustainability, and performance, spanning applications from micro-scale printable electronics to large-scale energy storage infrastructures.

ABSTRACTS OF INVITED SPEAKERS

Molecular lifetime, capacity fade and capacity recovery with organic active species

Prof. Dr. Michael J. Aziz

Harvard University

We have developed high performance flow batteries based on the aqueous redox behavior of small organic and metalorganic monomers composed of earth-abundant elements. These redox active materials can be inexpensive and exhibit rapid redox kinetics and high solubilities, potentially enabling rapid scaling of flow batteries at reduced cost. Adequate molecular lifetime has been one of the most challenging requirements to satisfy. We have shown that the amount of lost capacity is determined primarily by the molecular calendar life, which can depend on state of charge and temperature, but is independent of the number of charge-discharge cycles imposed. I will show how galvanostatic cycling introduces artifacts into capacity measurements that vitiate low fade rates based solely on galvanostatic cycling and will show how potential holds during cycling eliminate those artifacts, permitting the measurement of extremely low capacity fade rates. I will discuss how an understanding of molecular decomposition mechanisms has permitted us to design molecules with decadal projected lifetimes and even to reverse capacity fade by recomposing decomposed molecules within the functioning battery electrolyte.

ABSTRACTS OF INVITED SPEAKERS

Membrane-Free Redox Flow Batteries: Design Strategies and Performance Enhancement

Dr. Rebeca Marcilla

IMDEA Energy Institute

Redox flow batteries (RFBs) are promising candidates for large-scale energy storage due to their decoupled energy and power design, safety, and long cycle life. However, the reliance on ion-exchange membranes significantly increases system cost and can limit long-term stability due to crossover and degradation. In this talk, I will present recent advances in the development of membrane-free redox flow batteries, focusing on alternative design strategies that eliminate the need for costly separators while maintaining high performance.

Our approach is based on the rational design of organic electroactive materials combined with tailored electrolyte engineering, such as immiscible biphasic systems.^[1,2] Particular emphasis will be placed on current strategies to mitigate the inherent self-discharge at the liquid–liquid interface. These approaches enable effective spatial separation of redox species, suppress crossover, and enhance cycling stability.^[3,4]

Recent results demonstrate improved coulombic efficiency, extended cycling stability, and competitive energy densities, positioning membrane-free configurations as a viable pathway toward low-cost and sustainable energy storage technologies. The insights discussed provide general guidelines for the design of next-generation RFBs beyond conventional membrane-based architectures.

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ABSTRACTS OF INVITED SPEAKERS

Unlocking the second electron In the electrochemical delithiation/lithiation of *p*-DHT derivatives: Cu²⁺ effect

Prof. Dr. Steven Renault

French National Centre for Scientific Research

For *n*-type organic electrode materials, a particularly critical point is the very limited number of positive organic electrode materials that are prepared directly in their reduced state (eg. lithiated) for a Li-ion cell configuration.

In the last fifteen years, our lab has developed lithiated *p*-dihydroxyterephthalate-based (*p*-DHT) positive electrode material for Li-organic batteries, starting with dilithium (2,5-dilithium-oxy)-terephthalate salt (Li₄-*p*-DHT) using an original, solvent-free synthetic route.¹ Galvanostatic cycling delivered approximately one Li⁺ per formula unit corresponding to a reversible capacity of ~118 mAh g⁻¹ at an average potential of 2.55 V vs Li⁺/Li. The full two-electron theoretical capacity (241 mAh g⁻¹) was not achieved, since oxidation stalled before reaching the fully quinoid state. Instead, the material stabilized in a semiquinone radical intermediate, limiting practical capacity but defining a clear one-electron redox plateau.

Spectator-cation substitution offers an excellent, structure-preserving route to tune the electrochemistry of the *p*-DHT⁴⁻ redox center in the solid state by acting on coordination electrostatics rather than on the redox-active framework itself. In these salts, Li⁺ remains bound to the two phenolate oxygen atoms that host the reversible hydroquinone $\rightleftharpoons$ semiquinone $\rightleftharpoons$ quinone chemistry, while non-redox active "spectator" cations are deliberately chosen in the s-block.

Especially, Mg(Li₂)-*p*-DHT provides a reference framework for rationalizing the spectator-cation effect in this series of material.² Because of the large ionic potential of Mg²⁺, the Mg–O interaction shows an enhanced covalent character, which significantly reduces the donor inductive effect of the phenolate group conjugated with the aromatic ring, resulting in the increased operating potential observed during reversible Li⁺ extraction (~3.4 V), despite still being limited to a one-electron reaction.

Our recent extension of this concept from s-block spectator cations to a 3*d*-block (with Zn²⁺ and Cu²⁺)^{3,4} derivative demonstrates its extended validity. While bulk copper (2,5-dilithium-oxy)-terephthalate exhibits limited electrochemical activity when processed as a conventional powder electrode, direct synthesis of this material onto a high-surface-area conductive carbon scaffold enabled access to the second electrochemical process associated with oxidation of the phenolate units to the quinone form. This carbon-supported architecture ena-

ABSTRACTS OF INVITED SPEAKERS

bled specific capacities approaching the theoretical capacity for the complete two-electron redox process of the *p*-dihydroxyterephthalate framework ($\sim 190 \text{ mAh g}^{-1}$), corresponding to the extraction of nearly two lithium ions per formula unit at an average operating potential close to 3.5 V vs Li^+/Li .

Moreover, the integration of magnesium- and zinc-based (2,5-dilithium-oxy)-terephthalate positive electrodes with polyester-based solid polymer electrolytes was investigated, as well as a recycling route for $\text{Mg}(\text{Li}_2)$ -*p*-DHT electrodes. A reprotonation step enabled regeneration of the parent organic precursor 2,5-dihydroxyterephthalic acid, together with the recovery of lithium and magnesium as corresponding salts.

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ABSTRACTS OF INVITED SPEAKERS

Sustainable stretchable organic batteries for wearable electronics

Nara Kim^{1*}, Aiman Rahmanudin¹, Danfeng Cao¹, Jong Won Lee², Myung Han Yoon², Klas Tybrandt¹

¹Laboratory of Organic Electronics, Department of Science and Technology (ITN), Linköping University, Bredgatan 33, Norrköping, Sweden

²School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Gwangju 61005, Republic of Korea

nara.kim@liu.se

Driven by the need for sustainable energy storage, organic batteries based on renewable materials have attracted increasing attention. Beyond sustainability, organic materials offer additional advantages, such as mechanical flexibility and potential biocompatibility—key requirements for wearable and bio-integrated electronics that operate under deformation and in contact with biological environments. However, despite these benefits, the development of organic batteries has largely focused on conventional architectures, and their potential for wearable applications remains underexplored. In particular, stretchable organic batteries capable of maintaining stable electrochemical performance under mechanical deformation are still at an early stage.

Here, we present recent advances in stretchable organic batteries enabled by several design strategies¹: (i) stretchable composite electrodes with redox-active molecules embedded in an ion-conducting elastomer matrix², (ii) stretchable porous electrodes infiltrated with redox molecule-containing gel electrolytes^{3,4}, and (iii) flowable paste-like electrodes based on redox polymer nanoparticles and conductive networks⁵. These electrodes are integrated with various stretchable separators and current collectors to achieve mechanically compliant full cells with stable electrochemical performance under repeated mechanical deformation. These emerging battery systems hold strong potential for ubiquitous wearable electronics, including IoT sensors for continuous human and plant health monitoring, and may further enable low-cost, disposable or transient electronic applications.

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ABSTRACTS OF INVITED SPEAKERS

From milliwatts to megawatts: Bringing an organic flow battery technology to scale

Dr. Tobias Janoschka

Jena Flow Batteries GmbH

How does a battery technology move from molecular design in the laboratory to large-scale energy storage in the field? This presentation explores the scale-up journey of an organic flow battery technology, based on TEMPO chemistry, from its scientific beginnings roughly a decade ago to systems in the MWh range today.

The story begun with the identification and development of suitable organic active materials and continued through the first laboratory prototypes, increasingly advanced demonstrators and the world's first organic flow battery deployed in the field in 2019. From there, the technology progressed towards larger and more demanding applications reaching installations of up to 20 MWh in 2025.

At the heart of this journey is a key insight: successful battery innovation is not achieved by chemistry alone. Flow batteries store energy in liquid electrolytes held in external tanks and convert it in an electrochemical stack, enabling the independent scaling of energy and power. This unique architecture creates major opportunities for long-duration stationary storage (LDES), but it also makes scale-up a true multidisciplinary challenge. Promising molecules must be transformed into robust, reliable and economically viable systems that perform under real operating conditions.

In this context, the presentation highlights how the focus shifted during scale-up from electrochemical feasibility to system performance and from material selection to manufacturability. Selected examples will illustrate how scientific progress and practical implementation must come together to unlock commercial relevance.

It concludes with an outlook on the next phase of development and the role such systems can play in enabling resilient, safe and scalable energy storage for the energy transition.

ABSTRACTS OF INVITED SPEAKERS

Three-dimensional morphology of polymer-based batteries: Combining tomographic 3D imaging with modeling and simulation

Dr. Ingo Manke

HZB für Materialien und Energie

The 3D morphology of battery electrodes is a crucial factor for their performance and degradation behavior. Ensuring simultaneous ionic and electronic conductivity requires an optimal hierarchical 3D structure on the micro- and nanometer scales. Therefore, accurate knowledge of this morphology is indispensable to improve polymer-based batteries.

This talk provides an overview of recent developments in the analysis, modeling, and simulation of polymer-based battery electrode materials to better understand their structure-property-fabrication relationships. Advanced imaging techniques, such as FIB/SEM and synchrotron X-ray tomography, are used for detailed multiscale analysis. A main challenge is separating the 3D distribution of different materials within the complex mixture of redox-active polymers, conductive carbon, and binders. Through AI-supported statistical 3D image analysis, correlations between fabrication parameters and transport-relevant morphological descriptors of pristine and aged electrodes are quantified. This information feeds into spatially resolved numerical transport simulations using a multiscale electrochemical model. Finally, some results on the creation of virtual 3D morphologies by Generative AI will be demonstrated. This enables the systematic, cost-effective study of electrode microstructures (Virtual Materials Testing and Design).

Altogether, combining 3D imaging with model-based simulation generates design recommendations to optimize the electrochemical performance of polymer-based battery electrodes.

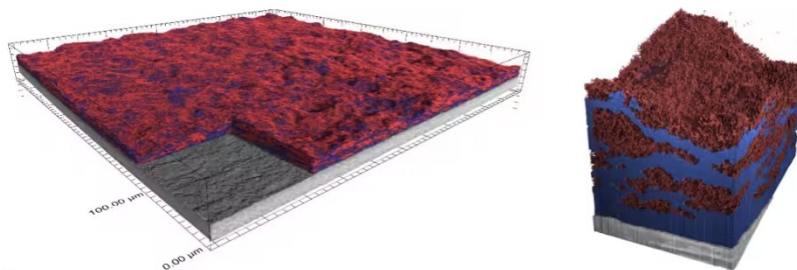


Fig.1: Tomographies of polymer-based battery electrodes

ABSTRACTS OF INVITED SPEAKERS

Challenges and experiences from commercializing organic flow batteries

Dr. Cedrik Wiberg

Rivus Batteries GmbH

The talk will cover Cedrik's academic career, founding Rivus as well as challenges and experiences of transitioning from academia to industry. The type of research that is done in a startup in order to quickly develop and commercialize a technology has enormous benefits as well as constraints compared to university research. This talk will focus on Rivus' R&D journey, mistakes and successes as well as which aspects of Rivus' R&D were the most important. Finally, the talk will cover techno-economics and experiences from scaling up the production and supply chain of organic energy storage molecules.

ABSTRACTS OF INVITED SPEAKERS

Molecular design of high-potential PROXYL radicals for advanced organic batteries

Nerea Casado,^{1,2} Gabriele Lingua,¹ Laura Pastor-Muñoz,³ Eduardo Sanchez-Díez³

¹ POLYMAT, University of the Basque Country UPV/EHU, 20018 Donostia-San Sebastian, Spain.

² IKERBASQUE, Basque Foundation for Science, E-48011, Bilbao, Spain

³ CIC energiGUNE, Parque Tecnológico de Alava, Albert Einstein 48, 01510, Miñano, Spain

nerea.casado@ehu.eus

The development of high-energy-density organic batteries relies on redox-active materials that combine fast electron-transfer kinetics, structural tunability, and sustainable design principles. Among the most promising classes of compounds, organic radicals have emerged as highly versatile redox materials due to their reversible one-electron chemistry, high redox kinetics, and molecular design flexibility.^[1] These characteristics have enabled their successful implementation in both redox flow batteries and Li-organic battery technologies, offering opportunities for scalable energy storage based on organic active materials with tunable electrochemical performance. However, further improvements in operating voltage remain a key challenge to fully unlock their potential for high-energy applications.

In this talk, we present our recent advances in the design of PROXYL-based radical systems as a new platform to increase the redox potential of organic electrodes beyond the limits of conventional nitroxide chemistries. By rational molecular engineering of the PROXYL scaffold we have developed a redox polymer, poly(PROXYL methacrylate), for Li-organic batteries,^[2] as well as catholyte materials for Aqueous Organic Redox Flow Batteries (AORFBs)^[3]. We have successfully shifted the redox potential to significantly higher values while preserving the fast and reversible electron-transfer characteristics that define stable organic radical batteries (ORBs). The combination of high redox potential, good cycling stability, and processability demonstrates the potential of PROXYL chemistry to expand the energy density of organic batteries.

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Abstracts of Oral Contributions

ABSTRACTS OF ORAL CONTRIBUTIONS

The impact of electrolyte formulation on the electrochemical performance of PTMA-based electrodes

Xiao Yao^{1,2}, Christian Friebe³, Ulrich S. Schubert^{1,4}, Andrea Balducci^{1,2,*}

¹ Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany

² Institute for Technical Chemistry and Environmental Chemistry, Friedrich Schiller University Jena, Jena, Germany

³ Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Jena, Germany

⁴ Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany

* andrea.balducci@uni-jena.de

Poly(2,2,6,6-tetramethylpiperidiny-N-oxymethacrylate) (PTMA) is among the most promising cathodic materials for organic radical batteries. In this study, we considered the impact of the electrolyte formulation on the electrochemical performance of this material.

Specifically, we investigated the use of the fluorine-free ionic liquid 1-butyl-2,3-dimethylimidazolium bis(oxalato)borate (BDMimBOB) in combination with acetonitrile (ACN), γ -butyrolactone (GBL) and γ -valerolactone (GVL). We showed that the solvent selection plays a decisive role on the electrode and devices performance. In fact, although the ACN-based electrolyte has the highest ionic conductivity, its use has a negative impact on electrode stability. In contrast, the use of a GBL-based electrolyte enables good current performance and excellent cycle stability (98% capacity retention after 500 cycles at 1 C).

Based on these results, hybrid devices containing a PTMA-based positive electrode and an activated carbon (AC)-based negative electrode were subsequently assembled, using GBL-based electrolytes. We showed that these systems display high energy density (up to 30 Wh kg⁻¹), good rate capability and high cycle stability (capacity retention of 70% after 500 cycles at 1 C). These results demonstrate the combined use of BDMimBOB and GBL represents a promising strategy for the realization of high performance PTMA-based energy storage devices.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Bipolar molecules and posolytes for aqueous organic flow batteries: Exploring new chemistries for different pH

Carlo Cajaniello¹, Darius Pakarinen^{1,2}, Julius Kuzmin³, René Wilhelm⁴, Mårten Ahlquist³, Amirreza Khataee², Helena Lundberg¹

¹ Division of Organic Chemistry, Department of Chemistry, KTH Royal Institute of Technology, Teknikringen 30, SE-100 44 Stockholm, Sweden

² Division of Applied Electrochemistry, Department of Chemical Engineering, KTH Royal Institute of Technology, Teknikringen 42, SE-100 44 Stockholm, Sweden

³ Division of Theoretical Chemistry & Biology, Department of Chemistry, KTH Royal Institute of Technology, Teknikringen 14, SE-100 44 Stockholm, Sweden

⁴ Institute of Organic Chemistry, TU Clausthal, Leibnizstraße 6, 38678 Clausthal-Zellerfeld, Germany

Aqueous flow batteries (FBs) offer a safe, scalable, and potentially cost-effective solution for large-scale energy storage. Organic FBs (OFBs) have the dual advantages of using readily available elements (unlike vanadium-based systems) and relatively easy tunability of the organic electrolytes. Through molecular engineering, OFB electrolytes can be optimized for both cost and performance, though challenges regarding energy density and stability remain.^{1,2}

Organic redox-active molecules (ORAMs) are classified as negolytes, or negative electrolytes, posolytes, or positive electrolytes, or bipolar if they can act as both. Although posolytes often dictate overall battery performance, their development lags behind that of the negolyte.³ When designing new ORAMs, among other factors, the targeted operational pH of the electrolyte solution plays a key role, as it affects not only the stability and the solubility of the organic molecule but also the choice of its functionalization.⁴ Aqueous FBs can operate from acidic to alkaline pH; the former is typical of vanadium-based systems, while the latter is more commonly employed with organic compounds such as quinones as negolytes.⁵ At alkaline pH, the reference posolyte compound is the inorganic potassium ferrocyanide, whose stability is still debated,⁵ while at neutral pH, ferrocene and tempo derivatives are well-known.⁶

This work focuses on the development process, i.e., design and synthesis, of new ORAMs while targeting different operating pH values. The first part of the work focuses on the evolution of triarylaminines into a new family of bipolar molecules via the tethering of viologens while targeting pH-neutral aqueous flow batteries.^{7,8} The second part of the work explores the use of new functionalization strategies on imidazoles for the synthesis of new posolytes to achieve a fully organic alkaline FB. Synthetic accessibility, solubility, and redox performance are key criteria for the whole investigation.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Molecular insights into charge transport in conjugated radical batteries

Clara Zens¹, Christian Friebe², Stephan Kupfer¹

¹ Institute of Physical Chemistry, Friedrich Schiller University Jena, Helmholtzweg 4, 07743 Jena, Germany

² Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

clara.zens@uni-jena.de

Stable organic radicals are promising charge-storage materials for organic batteries. However, their lack of intrinsic electronic conductivity necessitates the use of conductive additives, which reduce the achievable specific capacity.^[1] To overcome this limitation, a recent joint theoretical-experimental effort developed a novel electrode material by combining stable organic radicals with a conductive polymer backbone.^[2,3] In this approach, the tetramethylpiperidiny-N-oxyl (TEMPO) radical is covalently linked to a polythiophene backbone via an amide linker.

Focus is set on the molecular dynamics and quantum mechanical modelling of charge transport (CT) processes in this electrode material.^[3] Recent work has evaluated two complementary aspects: CT within the polymer and CT of the electrolyte. The first aspect comprises the efficiency of intra- vs. intermolecular CT processes. Representative environmental configurations were obtained from molecular dynamics, while electronic couplings within selected microenvironments were analyzed using time-dependent density functional theory. These couplings served as descriptors of CT efficiency and demonstrated that the direct attachment of TEMPO to a polythiophene backbone provides a significant advantage over conventional TEMPO-based electrode materials relying on conductive additives.^[3] The second aspect comprises the influence of electrolyte transport on electrode's performance. Molecular dynamics were employed to determine electrolyte diffusion rates and radial distributions relative to the polymer. This way, experimentally observed differences in rate capability in different electrolyte systems were rationalized on a molecular level. Overall, our studies demonstrate how multiscale computational modelling can yield fundamental mechanistic insights and guide the rational design of high-performance conjugated radical batteries.

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ABSTRACTS OF ORAL CONTRIBUTIONS

First-principles and machine learning strategies for modeling organic batteries

Daniel P. Tabor¹

¹ Department of Chemistry, Texas A&M University

daniel_tabor@tamu.edu

Organic redox-active polymers offer a promising pathway towards sustainable energy storage because their molecular structures can be tuned over a broad chemical space. Realizing this potential requires predictive computational methods that connect molecular design with experimentally measurable battery performance across multiple length scales.

Our work combines electronic structure theory, molecular simulation, and machine learning to accelerate the discovery and understanding of redox-active polymers. We first developed machine-learning-assisted virtual screening workflows to identify potential low-potential, redox-active building blocks. Building upon these molecular discoveries, we developed multiscale machine learning and surrogate models to predict electron-hopping, ion transport, and charge storage properties in polymer electrodes. Close collaboration with experimental groups has enabled direct comparison between theory and experiment across a diverse set of polymer chemistries. Our computational methods have helped explain how linker length, polymer microstructure, tacticity, and electrolyte environments govern charge-transfer kinetics, swelling, and battery performance. This has helped establish general design principles for the next generation of organic electrode materials.

Finally, we will discuss ongoing efforts to integrate first principles simulations, machine learning, and high-throughput electrochemical measurements to accelerate the discovery and optimization of existing battery materials through tighter coupling between experiment and theory.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Computational exploration of structure-property relationships in redox-active organic materials

Doreen Mollenhauer^{1,2}

¹ Helmholtz Institute for Polymers in Energy Applications Jena

² Friedrich Schiller University Jena

doreen.mollenhauer@helmholtz-berlin.de

The development of redox-active organic materials with tailored electrochemical properties is crucial for advancing polymer-based batteries and organic redox-flow batteries. Computational methods facilitate the identification of promising candidates and provide insight into how structural modifications affect their electrochemical properties ^[1]. We developed a multistep screening approach that combines conformational sampling, extended tight-binding methods, and density functional theory (DFT) to predict redox potentials across different classes of compounds ^[2]. Experimental data and highly correlated wave-function-based calculations were used as benchmarks to evaluate the accuracy of these calculations.

The methodology was applied to viologen-inspired compounds in which heteroatoms, linkers, and electron-donating or electron-withdrawing substituents were systematically varied. This allowed us to identify structure-property relationships and derive molecular design rules for tuning redox potentials to be derived. Additional studies on quinone derivatives and dihydroxyphthalazines showed that, besides conventional substituent effects, hydrogen-bond formation, steric effects, and structural and energetic differences between relevant conformers can significantly influence the redox potentials ^[3]. Furthermore, simple geometric descriptors were introduced to estimate the general stability of quinone derivatives.

Overall, these studies demonstrate how quantum-chemical calculations can complement experimental material development by rationalizing molecular trends and by supporting the design of tailored organic electrode materials.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Molecular Insights into Capacity Fade in Non-Aqueous Redox Flow Batteries

Wenlong Tang², Jelte Steen², Johan Hjelm², Edwin Otten¹

¹ University of Groningen

² Technical University of Denmark

edwin.otten@rug.nl

The use of organic active materials in redox flow batteries (RFBs) presents a promising approach to sustainable large-scale energy storage. However, the cycling stability of organic RFB electrolytes is generally limited by the occurrence of degradation reactions that cause capacity fade ^[1]. These reactions are commonly thought to form organic products that are no longer electrochemically active.

Here we study capacity fade in non-aqueous RFBs using an organic radical based on the 1,2,4-benzotriazin-4-yl ('Blatter' radical) scaffold ^[2,3]. The bipolar character of these radicals allows construction of symmetrical RFBs (i.e., with identical posolyte and negolyte composition) that do not suffer from crossover-induced capacity fade. This provides access to the determination of intrinsic electrolyte stability features that were previously hidden.

Our long-term cycling data shows that after an initial period of stable cycling (several days), the capacity fade rate increases in an autocatalytic fashion. Using (in-situ) spectroscopy and electrochemistry measurements, we trace this behavior to acid-catalyzed decomposition of the PF6⁻ supporting salt anion rather than active material degradation. We demonstrate that this is a universal, previously overlooked contributor to capacity fade in non-aqueous RFBs with commonly used PF6⁻ supporting salts. By replacing PF6⁻ with other anions, the stability of these non-aqueous electrolytes was substantially improved. Taking advantage of this insight, we demonstrate a symmetrical organic RFB that combines high energy- and current-density with excellent long-term cycling stability.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Diagnosing performance-limiting factors in Fe-AQDS redox flow batteries

Emilio Avellone^{1,2,3}, Sarah Ronchetti^{1,2,3}, Thomas R. Goodwin², John N. Vergados², Jennifer L. M. Rupp^{1,4}, Fikile R. Brushett^{2,3}

¹ Technical University of Munich, Munich, Germany

² Massachusetts Institute of Technology, Cambridge, USA

³ TUM Institute for Advanced Study, Garching, Germany

⁴ Fritz Haber Institute of the Max Planck Society, Berlin, Germany

emilio.avellone@tum.de; emilioav@mit.edu; brushett@mit.edu

Redox flow batteries (RFBs) are promising electrochemical systems for long-duration energy storage due to their independent scaling of power and energy, long operational lifetimes, simple manufacturing, and potential compatibility with low-cost and environmentally friendly active species ^[1]. Aqueous iron-anthraquinone disulfonic acid (AQDS) batteries combine an abundant inorganic redox couple with a low-cost organic active material and have been identified as a promising alternative RFB chemistry by many ^[2,3]. However, detailed characterization of their performance and usage remains limited.

Here, we diagnose the main performance-limiting factors of hydrochloric acid-based Fe/AQDS flow batteries through cycling of symmetric and asymmetric cells, complemented by ex situ characterization. We first show that AQDS cycling stability is highly sensitive to oxygen exposure: cells operated under conventional inert-gas blanketing exhibit a reproducible failure after approximately 50 h, whereas rigorous oxygen exclusion (i.e., <150 ppm O₂ environment) suppresses this failure mode. Under oxygen-free conditions, full cells remain operational for at least one week but display a progressive capacity decrease. Capacity recovery upon electrolyte rebalancing, together with ex situ quantification of Fe in the AQDS electrolyte, links this decay to Fe crossover through the membrane, Nafion 117, and the resulting active-material imbalance. Finally, in a symmetric mixed-electrolyte configuration, with Fe and AQDS present on both sides of the cell, capacity is maintained over one week of cycling (~100 cycles). These results identify oxygen exposure and crossover-induced imbalance as the dominant performance limitations of acidic Fe/AQDS flow batteries and establish practical conditions for their reliable evaluation and operation.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Indolocarbazole: A high-voltage multi-electron p-type redox center for organic electrode materials

Ji Eon Kwon¹

¹ Korea Institute of Science and Technology

jekwon@kist.re.kr

Organic electrode materials (OEMs) have attracted considerable attention as promising alternatives to conventional inorganic electrode materials for secondary batteries due to their advantages, including abundance, sustainability, potential biocompatibility, cost-effectiveness, and chemical tunability. However, most reported OEMs based on n-type redox centers exhibit relatively low charge/discharge voltages (<3.0 V vs. Li/Li+), compared with their inorganic counterparts. Recently, numerous high voltage OEMs (>3.5 V vs. Li/Li+) have been reported relying on a limited number of p-type redox centers such as dihydrophenazine, phenoxazine, and phenothiazine.^[1] Nevertheless, the narrow electrochemical window of conventional electrolytes often prevents access to the higher oxidation states required for multi-electron redox reactions, thereby limiting the attainable specific capacity.

In this talk, we present dihydroindolocarbazole (ICZ), in which two carbazoles are fused through a central phenyl ring, as a new p-type redox center for high energy density cathode materials. Notably, 5,11-diethyl-5,11-dihydroindolo[3,2-b]carbazole (DEICZ) undergoes two single-electron redox reactions at high potentials of 3.44 and 4.09 V vs. Li/Li+ within the stable electrolyte window, leading to high theoretical capacity.^[2] To improve the cycle stability, vinyl groups capable of in situ electrochemical polymerization is introduced, which effectively suppresses active material dissolution and allows stable cycling over several hundred cycles.^[3] Then, we further explore the electrochemical properties of positional ICZ isomers in which the two N atoms are arranged in para, meta, or ortho configurations relative to each other.^[4] Interestingly, the redox potentials, cycle stability, and rate capability of the ICZ isomer electrodes can be systematically tuned depending on the N positions.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Conjugated sulfonamides for next generation energy storage

Jiande Wang¹, Alae Eddine Lakraychi¹, Xiaolong Guo¹, Robert Markowski¹, Alexandru Vlad¹

¹ College of Materials Science and Engineering, Hunan University, China

jiandewang@hnu.edu.cn

50 years ago, pretty much at the same time when the first man walked on the Moon, battery scientists were also developing the first organic battery! Whereas space science has “rocketed” since, organic batteries, and in general, the battery field, has seen less disruptive advances. Over the past 2 decades however the organic battery field has seen a renaissance, most certainly driven by the sustainability and the raw materials criticality concerns for the upcoming massive battery demand. However, despite all this effervescence, a key component remains underdeveloped in the organic battery value chain: the organic metal-ion positive electrode chemistries with practical characteristics - resistant to oxidation and hydrolysis in ambient air in the reduced, metal-ion reservoir form, alike the conventional metal-ion cathodes. In this talk, I will broadly debate the possibilities for development of new organic redox chemistries with high voltage, ambient air stability in the metal-ion reservoir form, and intrinsic electrical conductivity. Some of the designed organic chemistries are also found to store not only the monovalent cations, but also highly efficient for the divalent cation storage, with extension to high voltage electrolytes and all solid-state systems by designing functional mixed ion-electron conducting battery materials ^[1-5].

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ABSTRACTS OF ORAL CONTRIBUTIONS

Advanced organic polymer electrodes for lithium and sodium-ion batteries

Jonathan Caroni^a, Arindam Mal^a, Asia Patriarchi^b, Jon Otegi^c, Leonardo Sbrascini^d, Hegoí Manzano^c, Olivera Luzanin^e, Rafael Ramos^a, Manuel Melle Franco^f, Jan Bitenc^e, Javier Carrasco^g, Miguel Ángel Muñoz Márquez^d, Manuel Souto^a

^a Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS), Departamento de Química-Física, Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain

^b Chemistry Division, School of Science and Technology, University of Camerino (UNICAM), Via Madonna delle Carceri-ChIP, 62032 Camerino, MC, Italy

^c Department of Physics, University of the Basque Country (UPV/EHU), Sarriena auzoa, z.g., 48940 Leioa, Spain

^d International Iberian Nanotechnology Laboratory (INL), Avenida Mestre Jose Veiga, 4715-330 Braga, Portugal

^e National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

^f Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-393 Aveiro, Portugal

^g Centre for Cooperative Research on Alternative Energies (CIC Energigune), Basque Research and Technology Alliance (BRTA), Araba Technology Park, Albert Einstein 48, 01510 Vitoria-Gasteiz, Spain

j.caroni@usc.es

Lithium-ion batteries are a key technology for renewable energy storage and electric mobility, but rely on critical raw materials such as Li, Co, and Ni, raising sustainability and supply concerns. In this context, organic electroactive materials have emerged as promising alternatives to conventional inorganic electrodes. Based on abundant elements (C, O, N, S), they offer environmental advantages, high theoretical capacities, and tunable electrochemical properties through molecular design. A common strategy to improve cycling stability is the polymerization of redox-active units to suppress dissolution in the electrolyte. Covalent Organic Frameworks (COFs) are particularly attractive due to their ordered porosity and designable redox sites, and are increasingly explored for sodium-ion batteries, which benefit from the natural abundance of sodium. However, despite these advantages, suitable electrode materials for sodium storage are still limited, highlighting the need to better understand their charge storage mechanisms.

We first report a novel organic polymer as a high-capacity cathode for lithium-ion batteries, where in situ growth on carbon nanotubes overcomes the intrinsically poor electronic conductivity of the polymer.^[1] We then investigate the sodium storage mechanism in a redox-active COF cathode for Na-metal batteries. Molecular dynamics simulations combined with ex situ X-ray diffraction analyses reveal that sodium ions are primarily stored through interactions with car-

ABSTRACTS OF ORAL CONTRIBUTIONS

bonyl groups within the COF channels, rather than via interlayer intercalation. Finally, we systematically evaluate, for the first time in COF-based electrodes, the effect of calendaring through combined electrochemical and structural characterization.^[2]

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ABSTRACTS OF ORAL CONTRIBUTIONS

Synthesis of organic macromolecular materials for solid organic batteries

Julie Schulz^{1,2}, Matthieu Becuwe^{1,2}, Sébastien Gottis^{1,2}

¹ Université de Picardie Jules Verne, Laboratoire de Réactivité et Chimie des Solides (LRCS, UMR CNRS 7314), 80000 Amiens, France

² Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, 80039 Amiens, France

julie.schulz@u-picardie.fr

Over the past decades, organic materials have shown tremendous advantages in batteries. Indeed, raw materials abundancy of and cost-effective due to low energy consumption in synthesis paths are one of them. Nevertheless, organic electrode materials encounter challenges among which are their solubility in organic electrolytes and low ionic and electronic conductivity. This deficiency leads to lower electrochemical performances comparatively to their inorganic alternatives and requires a higher amount of conductive carbon. The solubility of the organic electrodes leads to a quick fading in terms of capacity and life-time expectancy. Recently, macromolecular electrode gained attention due to the excellent properties of THAQ (hexakis(2-anthraquinonyloxy) cyclotriphosphazene) which demonstrated high discharge capacity of 114 mAh/g with a retention capacity of 82.5% after 1000 cycles and a high coulombic efficiency.^[1] Triazine based dendritic structures were investigated as well, as they enhance the charge storage and the transport of lithium ions, achieving specific capacity of 444-500 mAh/g after 200 cycles.^[2] In this context, our work focuses on the development of a versatile coupling platform, and can host up to six electroactive groups. Different redox active groups such as quinones, phenothiazines, TEMPO have been carefully selected for this study. At first, we synthesized several new macromolecular redox active materials for lithium ion batteries with controlled solubility thanks to a hyperbranched structure. Then after, we focused our attention on investigating, physical and electrochemical activities of our new redox active organic material.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Polymers to stabilize the supercooled liquid state of Li salts: An approach to organic solid state batteries

Kenichi Oyaizu¹, Akinari Chiba¹, Toshinori Kozakai¹, Yuki Ogawa¹

¹ Department of Applied Chemistry, Waseda University

oyaizu@waseda.jp

Developing safe batteries poses the critical challenge of finding solid electrolytes with high ionic conductivity and electrochemical stability. Although various materials, such as oxides and sulfides, have been investigated for use in lithium-ion batteries, improvements are still needed for all-solid-state batteries. However, a lack of understanding of electron and ion transport within the solid electrolyte and at the electrode interfaces hinders further progress. The same applies to solid polymer electrolytes (SPEs), which use polymers as their main component. SPEs have attracted attention due to their potential to reduce interfacial resistance based on their inherent adhesion and moldability. However, their conductivity levels are still two to three orders of magnitude lower than required for practical applications. Polyethylene oxide (PEO) derivatives are the most extensively studied SPEs. Although these derivatives effectively dissolve Li salts, the diffusion of Li ions is significantly restricted by the segmental motion of the coordinated PEO chains. In contrast, the polymer-in-salt type of SPEs was proposed ca. 30 years ago as a groundbreaking method capable of overcoming the conductivity limit ^[1]. In these SPEs, the composition is reversed, incorporating a small amount of PEO into the Li salt. Since then, many examples of polymers constituting such SPEs have been reported, which are thought to exhibit conductivity by stabilizing the supercooled liquid state of Li salts. Here we report that polymer-in-salt SPEs composed of aliphatic poly(thio)ethers and related polymers exhibit a high conductivity of 10^{-4} S/cm ^[2,3]. These SPEs also possess the mechanical strength necessary to form self-standing films. This gives rise to the performance of all-organic solid-state batteries based on their excellent interfacial contact with organic electrodes.

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ABSTRACTS OF ORAL CONTRIBUTIONS

How “Green” is your functional material? Assessing environmental impacts of multi-step synthetic protocols in material sciences at various technology levels

Laura Plein^{1,§}, Alexander Schommer^{2,§}, Florian Dietrich^{1,2}, Moritz Gutsch², Heike Klesper¹, Kevin Schuller¹, Lars Jahnke², Jens Leker^{2,3}, Klaus Meerholz^{1,*}

¹ Department of Chemistry and Biochemistry, University of Cologne, Greinstrasse 4-6, 50939 Cologne, Germany

² Institute of Business Chemistry, University of Münster, Leonardo-Campus 1, 48149 Münster, Germany

³ Helmholtz Institute Münster, IEK-12, Forschungszentrum Jülich GmbH, 48149 Münster, Germany

klaus.meerholz@uni-koeln.de

Environmental awareness is increasing worldwide, driven by alarming developments such as the climate change. Therefore, counteractions to slow down or even reduce these negative impacts have been undertaken. Life cycle assessment (LCA) provides a standardized framework to evaluate environmental impacts. Here, we introduce a broadly applicable formalism referred to as Environmental Synthesis Radar (ESR) to systematically evaluate the environmental impacts of multi-step chemical synthesis protocols ^[1]. ESR goes beyond the typical consideration of only one particular environmental aspect (e.g. “global warming”), but rather considers 18 midpoint impact categories (MICs), and thus yields a much more holistic and conclusive view. Normalization of the individual impacts to the global annual environmental emissions per capita, i.e., the worldwide annual environmental emissions divided by the world's population, enables comparability of results across different MICs and facilitates contextualized interpretation. We obtain three important environmental metrics: (i) the per capita annual environmental output V_{total} , a single number for comparison of different materials and contextualized interpretation; (ii) the environmental fingerprint VEF for identification of the most impactful MICs, and (iii) the process radar VPR, which allows identification of environmentally critical synthesis steps and substances. Exemplarily, the ESR formalism is applied to two cathode material classes for use in secondary batteries: an organic material based on tris-(p-methoxy)-phenylamines (TPA) and an inorganic reference based on lithiated nickel-manganese-cobalt oxide (NMC). ESR indicates that the impact of synthesizing 1 kg of these materials is a factor of 3 (TPA) or 18 (NMC) below the global annual environmental emissions per capita, demonstrating that the laboratory synthesis of TPA is about one order of magnitude more harmful than the industrial production of NMC.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Study of four electron exchange on benzene and naphthalene ring

Klemen Pirnat^a, Svit Menart^a, Vladyslav Yatsenko^{a,b}, Robert Dominko^{a,b,c}

^a National Institute of Chemistry, Hajdrihova 19 SI, 1000 Ljubljana, Slovenia

^b Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113 SI, 1000 Ljubljana, Slovenia

^c Alistore-European Research Institute, CNRS FR 3104, Hub de l'Energie, Rue Baudelocque, 80039 Amiens, France

klemen.pirnat@ki.si

Redox active organic materials are gaining interest as sustainable candidates for future energy storage. One of their main advantages are their high theoretical capacities up to 957 mAh/g (hexaketocyclohexane), which are much higher than their commercial inorganic materials (NMC and NCA 275 mAh/g, LFP 170 mAh/g, LCO 274 mAh/g). We focused on small 1,2,3,4-tetrahydroxybenzene with high theoretical capacity 755 mAh/g. We were able to chemically synthesize all three redox states: reduced (MH4), half oxidized (MH2) and fully oxidized (M) and then electrochemically convert one into another. In this way we indirectly proved it can undergo reversible 4 electron redox reaction. We have tested MH2 in several organic electrolytes and best reversibility was obtained in acidic aqueous media. For battery application we have also prepared polymer with 1,2,3,4-tetrahydroxybenzene redox pendant (RPN 3c), which was tested in Zinc (3M ZnSO₄ in H₂O electrolyte) and Lithium battery using several different organic electrolytes. In both cases, the obtained capacity was very low (low utilization) and dropped fast in a few cycles ^[1]. To improve the results, the idea was to develop an electronic conjugated polymer (electronic conductivity) with stronger π - π stacking (lower solubility) based on direct polymerization of 1,2,3,4-tetrahydroxynaphthalene (Fig. 1).

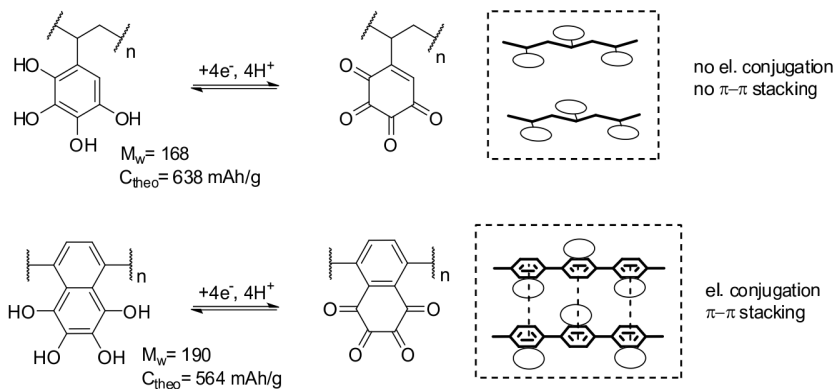


Fig. 1. Schematic representation of 1,2,3,4-tetrahydroxy redox center on benzene and naphthalene ring, corresponding polymers and their characteristics.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Electrochemical characterization of flow battery active materials: rotating disc electrode voltammetry vs. electrochemical impedance spectroscopy

Koosha Ehtiati^{a,b}, Christian Stolze^{a,b}, Taha Abdellatif^{a,b}, Philip Zimmer^d, Sebastian Witt^{a,b}, Kristin Schreyer^{a,b}, Martin D. Hager^{a,b,c,d,e}, Ulrich S. Schubert^{*a,b,c,d,e}

^a Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany

^b Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

^c Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Philosophenweg 7, 07743 Jena, Germany

^d Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstr. 12-14, 07743 Jena, Germany

^e Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

koosha.ehtiati@uni-jena.de

Organic redox-active molecules (ORM) have attracted remarkable interest for redox flow battery (RFB) applications. The electrochemical parameters of the ORMs, i.e. the heterogenous electron transfer rate constant (k_0) and the diffusion coefficient (D), directly influence the internal resistance of the RFB, and thus, accurate determination of such parameters is crucial.^[1]

Rotating disc electrode (RDE) voltammetry is a common method to characterize ORMs. However, the application of RDE for ORMs have drawbacks and pitfalls. The Koutecký-Levich equation that is typically used to determine the kinetic parameters is strictly applicable for electrochemically irreversible systems, while most ORMs show reversible or quasi-reversible behavior.^[2] Obtaining kinetic data based on RDE becomes more erroneous for the ORMs with fast electron transfer.^[3] Besides, RDE requires a long experiment time due to the relatively low scan rates applied to mimic steady state currents and the requirement for testing the supporting electrolyte to perform background subtraction.

Herein, we show that for ORMs with fast electron transfer the validity of the kinetic data obtained from RDE is questionable. Alternatively, a method based on electrochemical impedance spectroscopy (EIS) is proposed for characterization of ORMs. EIS is efficiently applied to the solutions of ORMs, and the kinetic and diffusion properties are obtained based on the resulting impedance spectra.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Life-cycle assessment of organic redox flow batteries for long-duration energy storage

Kristína Rabatinová¹, Atharva Kulkarni¹, Axel Fache⁴, Christian Stolze^{1,4}, Christian Friebe⁴, Martin Hager^{1,2,3,4}, Ulrich S. Schubert^{1,2,3,4}, Jacob Schneidewind^{1,2,3,4}

¹ Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany.

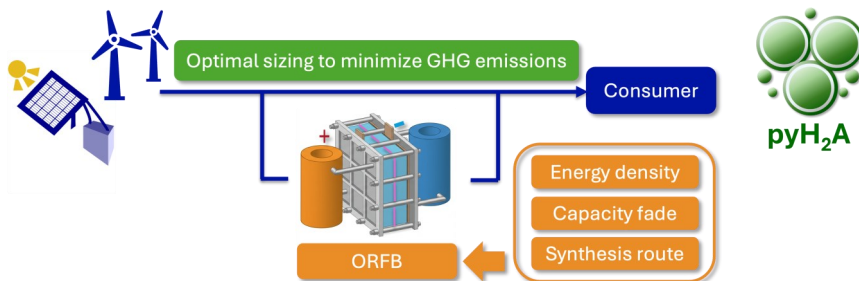
² Jena Center for Soft Matter (JSCM), Friedrich Schiller University Jena, Philosophenweg 7, 07743 Jena, Germany.

³ Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena.

⁴ Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany.

kristina.rabatinova@uni-jena.de

Development of sustainable, long-duration energy storage technologies (LDES) is essential for efficient use of variable renewable energy sources, such as wind or solar power. Organic redox flow batteries (ORFBs) are a promising class of LDES due to their scalability, intrinsic safety, and potential use of abundant, metal-free redox-active materials. However, their large-scale deployment remains constrained by sustainability and cost challenges. This study compares the sustainability of ORFBs to established technologies, such as vanadium flow and lithium-ion batteries, from a life-cycle perspective. The comparison is performed in the context of providing close to 100% renewable energy to large-scale electricity consumers, such as AI data centers, through the combination of wind power, solar power, and batteries. Special attention is paid to improvements to ORFB electrolyte chemistry, such as improvements in energy density, capacity fade, and sustainability of electrolyte synthesis route, impact the comparative life-cycle impacts. A Monte Carlo approach coupled with energy system optimization was chosen and calculations were performed using the open-source pyH2A modelling platform. Scenarios between the current state-of-the-art and future limits of ORFBs are explored. For each scenario, an energy system optimization is performed to identify the system configuration (wind, PV, battery sizing) that minimizes greenhouse gas emissions. The dataset provides quantitative insights into which electrolyte parameters most strongly impact the sustainability of energy storage. Furthermore, actionable targets for these parameters to surpass the environmental performance of vanadium flow and lithium-ion batteries are derived. This insights can guide research towards impactful improvements, ultimately leading to ORFBs that are suitable for large-scale, long-duration and sustainable energy storage.



ABSTRACTS OF ORAL CONTRIBUTIONS

Symmetric Aqueous Redox Flow Batteries and reference Ferri/Ferrocyanide pair: a critical look on the stability of ferrocene derivatives at neutral pH.

Leslie R. Arias-Arand^a, Anna M. Habak, William Er^b, Florence Mongin, Charlotte Bodin, Florence Geneste.

Institut des Sciences Chimiques de Rennes, Université de Rennes, Rennes, France.

leslie.arias@univ-rennes.fr

The global transition toward sustainable energy requires scalable, safe, and cost-effective energy storage systems, positioning aqueous organic redox flow batteries (AORFBs) as promising candidates for different applications at diverse scales.^{[1],[2]} Hence, AORFBs operating under environmentally friendly conditions at neutral pH remain a primary target; however, achieving long-time cycling stability under these conditions requires detailed analysis.^[3] In this work, we demonstrate the implementation of symmetric redox flow battery configurations as a reliable diagnostic tool to gain a deeper understanding of the intrinsic electrochemical stability of new water-soluble ferrocene derivatives. Through the analysis of the ferrocene derivatives at neutral pH, in comparison with the conventional and widely used standard of the ferri/ferrocyanide system, their stability is evaluated during extended charge and discharge cycling, evaluating the scope and accuracy of this standard reference. Moreover, the direct performance comparison shows that optimized ferrocene systems present highly competitive lifetime and electron transfer kinetics. Finally, our study highlights the essential role of using symmetric redox flow battery configurations, as well as reliable reference standards, to obtain accurate indicators of stability for ferrocene derivative molecules in AORFBs.

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ABSTRACTS OF ORAL CONTRIBUTIONS

A systematic study of hydroquinone dicarboxylate isomers for Li-ion batteries applications

Y. Zekhine, M. Nicolas, M. Claeys, P. Poizot, T. Gutel, and L. Dubois

Univ.Grenoble Alpes, CEA, CNRS, IRIG, SyMMES, 38000 Grenoble, France

lionel.dubois@cea.fr

Nowadays, electrodes of lithium batteries are mainly constituted by inorganic compounds based on transition metals, such as cobalt, nickel, or manganese. Whilst the performances of these materials are satisfactory, it must be noted that they are accompanied by several significant drawbacks. Eventually, their reactivity leads to safety issues in abusive conditions.

Organic electroactive compounds, such as nitroxide based polymers or carboxylate salts, offer a cost-effective and environmentally friendly alternative to conventional electrode materials for electrochemical storage. Interestingly, these products can be prepared from low-cost precursors using classical organic and polymer chemistry techniques. Moreover, these compounds are easy to recycle or reuse at their end of life. Eventually, organic electrode materials can follow N-doped but also P-doped redox mechanisms, which enable to imagine new battery configurations (cation-ion, dual-ion or anion-ion). But until now, their use is still challenging due to their low redox potential, the reactivity with air of their lithiated form, and low cycle life, usually related to their high solubility in organic solvents used as electrolytes.

Of all the redox organic compounds for battery applications, quinonoid derivatives are the most widely studied. Among these, p-dihydroxyterephthalic salts are the most promising, particularly the mixed magnesium–dilithium salt. This compound has one of the highest potentials (3.25 V/Li) of all lithiated quinone salts. In this presentation, I will present recent results obtained at CEA regarding the use and development of hydroquinone dicarboxylate isomers as positive electrode materials for lithium salts. The focus will be on synthesis, characterisation, and evaluation of their electrochemical behaviour.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Conductive positive electrode materials using molecular and material engineering

V. Pignier,^{a-c} M. Mignon,^{a-b} S. Toumieux,^c J.-N. Chotard,^{a-b} and M. Becuwe,^{a-b*}

^a. Laboratoire de Réactivité et de Chimie des Solides (LRCS), UMR CNRS 7314, Université de Picardie Jules Verne (UPJV), Amiens, 33 rue Saint-leu, 80039 Amiens, France

^b. Laboratoire de Glycochimie et des Agro-ressources d'Amiens (LG2A), Université de Picardie Jules Verne (UPJV), Amiens, 10 rue Baudelocque, 80039 Amiens, France

^c. Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, 80039 Amiens, France

matthieu.becuwe@u-picardie.fr

Over the past decade or so, organic electrode materials have emerged as serious contenders to replace traditional mineral-based electrode materials. Currently, their net performance even exceeds that of the much-vaunted LFP, which is making a comeback and is being positioned as a material of the future in light of current environmental, geopolitical and economic considerations.

However, organic materials still suffer from high solubility in the electrolyte and a lack of conductivity, which respectively limit the electrode's lifespan and restrict its energy density. Whilst the former issue can be satisfactorily addressed through the use of gelled or solid electrolytes, conductivity problems remain persistent and difficult to overcome.

With this in mind, several promising options have been explored by the research community, thereby opening up new avenues for progress towards the manufacture of competitive complete assemblies. These include the shift towards thin films,^[1] advanced electrode formulation - particularly for the negative electrode^[2] - and the design of materials with semiconducting or metallic properties through molecular engineering.^[3]

This latter approach has particularly caught our attention in recent years. The aim of this presentation is therefore to illustrate this approach by outlining two avenues which can lead to improved performance but which also present new challenges to be overcome.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Characterizing Sulfur–Organic Networks Formed by Inverse Vulcanization Using X-Ray Spectroscopy

Michael Walter

Freiburg Center for Interactive Materials and Bioinspired Technologies (FIT),
University of Freiburg, Georges-Köhler-Allee 105, 79110 Freiburg, Germany

Michael.Walter@fmf.uni-freiburg.de

Sulfur-rich copolymer networks prepared by inverse vulcanization offer a promising approach for stabilizing sulfur in lithium–sulfur batteries. While increasing the sulfur content can enhance the theoretical capacity, it also promotes the formation of long sulfur strands that are susceptible to lithium polysulfide formation, dissolution into the electrolyte, and subsequent deposition elsewhere in the cell, ultimately compromising long-term cycling stability.

Here, we address the influence of sulfur-strand length through sulfur K-edge near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. Theoretical predictions of NEXAFS spectra for model molecules are validated by experiment, showing near-perfect agreement on the absolute energy scale ^[1]. This agreement provides a reliable basis for interpreting NEXAFS spectra of real battery materials ^[2]. We apply this approach to sulfur-rich networks with systematically varied compositions. Longer sulfur strands increase the specific capacity but reduce cycling stability. In contrast, very short sulfur strands stabilize the specific capacity and exhibit excellent cycling stability over more than 1000 cycles ^[3]. These results demonstrate the potential of combining theoretical and experimental NEXAFS spectroscopy to characterize sulfur-network structures and relate sulfur-strand length to the electrochemical performance of inverse-vulcanized materials.

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ABSTRACTS OF ORAL CONTRIBUTIONS

From redox polymers to practical electrodes: Engineering high areal capacity in organic batteries

Nagaraj Patil, Rebeca Marcilla

Electrochemical Processes Unit, IMDEA Energy Institute, Avda. Ramon de la Sagra 3, 28935 Mostoles, Madrid, Spain

nagaraj.patil@energia.imdea.org

Organic electrode materials offer a sustainable and structurally versatile alternative to conventional inorganic electrodes, but their practical relevance is often obscured by testing thin electrodes with low active-material loading and large amounts of conductive carbon. This contribution presents a general electrode-engineering approach to move redox polymers from promising materials toward competitive battery electrodes by maintaining efficient electron and ion transport while increasing polymer content, electrode thickness and areal capacity.

In lithium cells, anthraquinone-based conjugated microporous polymer/nanocarbon hybrids were processed as self-standing, binder- and metal-current-collector-free electrodes. At 60 mg cm⁻² and only 20 wt% carbon, they delivered 6.3 mAh cm⁻² with stable cycling^[1]. The concept was then extended to readily available polyimides. Optimized polyimide electrodes reached 8.5 mAh cm⁻² at 55 mg cm⁻² and were translated from Li half-cells to graphite, LTO, LFP and NMC full cells, including pouch cells delivering 210 Wh kg⁻¹ and 32 mWh cm⁻²^[2]. Porosity and crosslinking also improved thick p-type phenothiazine polymer cathodes, reaching 3.85 mAh cm⁻²^[3].

The same principles are transferable to sodium-metal and aqueous alkaline batteries, where robust porous polymers sustain high areal output and long cycle life. These results show that molecular capacity alone is insufficient for judging organic electrodes. Areal and volumetric capacity, active-material fraction, electrode density, rate performance, electrolyte amount and full-cell balance must be considered together. Further progress requires higher redox-site density, lower carbon content, denser scalable architectures and realistic full-cell testing to close the gap with state-of-the-art inorganic batteries.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Electrochemical evaluation of extended viologens as negative electrode materials for anion-ion rechargeable batteries

Axel FLORENT, Thomas DEVIC, Stéven RENAULT, [Philippe POIZOT](mailto:philippe.poizot@cnrs-imn.fr)

Nantes Université, CNRS, Institut des Matériaux de Nantes Jean Rouxel, IMN, Nantes F-44000, France

philippe.poizot@cnrs-imn.fr

Among p-type organic redox systems, pyridinium-based electrophores represent a particularly attractive class of materials due to their reversible two-electron redox chemistry and readily tunable molecular structure. For instance, the 4,4'-bipyridinium motif (viologens) undergoes two consecutive one-electron reductions, providing access to three stable redox states and enabling efficient charge-storage processes. Importantly, the relatively low operating potentials of viologen derivatives distinguish them from many other p-type materials, making them promising candidates for negative electrodes in emerging anionic rocking-chair battery systems^[1,2]. In this contribution, we present a family of pyridinium-based electrophores, ranging from zwitterionic viologens and double salts to polymeric systems, developed as model platforms for studying anion-driven energy-storage mechanisms. Through a combination of molecular design, structural characterization, and electrochemical analysis, we explore how the ionic environment and molecular conformation, particularly the dihedral angle between pyridinium units, affect redox activity and tune the operating potential. These findings provide fundamental insights into structure-property relationships and offer new guidelines for the rational design of organic negative electrodes for anionic rocking-chair batteries.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Multiscale modeling of structural, ionic, and electronic properties of radical-containing polymers for all-organic batteries

Riccardo Alessandri¹, Kha Trinh², María Ley-Flores³, Daniel P. Tabor⁴, Stuart J. Rowan³, Jodie L. Lutkenhaus⁴, and Juan J. de Pablo²

¹Department of Chemical Engineering, KU Leuven, 3001 Leuven, Belgium

²Tandon School of Engineering, New York University, NY 11201, United States

³Pritzker School of Molecular Engineering, University of Chicago, Chicago, Illinois 60637, United States

⁴Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, Texas 77843,

United States

riccardo.alessandri@kuleuven.be

Solid-state electrodes built from radical-containing redox-active polymers as the active material offer an attractive route toward all-organic batteries. However, it remains unclear how the chemical structure of these redox-active polymers governs their performance, which limits further progress in the field.

In this presentation, I will describe our modeling efforts and how they inform, and are informed by, our experimental collaborators. Combining atomistic molecular dynamics, electronic structure calculations, and machine learning, we probe the structural, ionic, and electronic properties of a new class of phthalimide-containing redox-active polymers. We model a series of polymer-electrolyte systems, systematically varying the polymer backbone chemistry, electrolyte solution content, and state of charge. Our results ^[1] show that state of charge has a strong effect on solid-state packing and the polymers' thermo-physical properties, which in turn govern ionic and electronic transport. Together, molecular-level properties (e.g., reorganization energy) and condensed-phase properties (e.g., effective electron hopping distances) determine the predicted ranking of electron transport capabilities across the polymers.

I will conclude by discussing open challenges in bridging modeling and experiments, and opportunities brought about by methods that couple coarse-grained modeling with electronic structure prediction ^[2].

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ABSTRACTS OF ORAL CONTRIBUTIONS

Exploration of Quinone-Based Polymers for Organic Cathode Active Materials of Lithium-Ion Batteries

Rika Yamamoto,¹ Kosuke Sakano,¹ Taisei Sakata,² Shuntaro Miyakawa,²

Shino Yoshizaki,² Naoya Kobayashi,² Yasuhiko Igarashi,³ Yuya Oaki¹

¹ Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan

² Product Research & Development Division, Ubiquitous Network Planning Division, Technology Unit, SoftBank Corp., 1-7-1 Kaigan, Minato-ku, Tokyo 105-7529, Japan

³ Faculty of Engineering, Information and Systems, University of Tsukuba, 1-1-1 Tennodai, Tsukuba 305-8573, Japan

oakiyuya@applic.keio.ac.jp

Introduction: Exploration of high-performance cathode active materials is significant to achieve higher energy density. In a wide search space, efficient exploration method is required to find new active materials. In our previous works, combination of machine learning (ML) and chemical insight is an effective approach for exploration of new compounds and optimization of processes even on small data.¹⁾ The performance predictors for organic cathode active materials have been constructed.²⁾ In addition, amorphous conjugated polymer networks (CPNs) containing redox-active molecules were prepared by combining electrophilic substitution and pericyclic reactions.^{3,4)} Our intention here is to explore new high-performance cathode active materials using the performance predictor. Moreover, amorphous CPNs are synthesized by the discovered compounds using combinatorial polymerization technique.

Experimental: Commercially available three anthraquinone (**AQ**) derivatives were extracted by exploration using the performance predictor. Three homopolymers and 12 copolymers of the conjugated monomers and linkers were synthesized using combinational polymerization. After the screening charge-discharge measurements, electrode structures and compositions were optimized to enhance the performance.

Results & Discussion: The predicted capacity of **AQ1**, **AQ2** and **AQ3** was 413, 420, and 420 mA h g⁻¹, respectively. However, the monomers were dissolved in an electrolyte. Three homopolymers and 12 copolymers with benzoquinone (**BQ**), catechol (**Cat**), pyrrole (**Py**), and pyrazine (**Pz**) were synthesized based on **AQ1**, **AQ2**, and **AQ3**. The screening charge-discharge measurements of the homopolymers **AQ1** (**P(AQ1)**), **AQ2** (**P(AQ2)**), and **AQ3** (**P(AQ3)**) and copolymers **AQ3** were performed by preparation of the electrodes with acetylene black as a conductive carbon. Two compounds, **P(AQ3)** and **Py-AQ3**, showed the redox reactions over 2.5 V (vs. Li/Li⁺) and high capacity 130 mA h g⁻¹ and

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60.0 mA h g⁻¹ at 50 mA g⁻¹, respectively. FT-IR and Raman spectra showed the broadened peaks indicating the polymerization of **P(AQ3)** and **Py-AQ3**. The absorption peaks were assigned to the specific functional groups and chemical bonds originating from the **AQ3** units. The structures of **P(AQ3)** and **Py-AQ3** were estimated from ¹³C NMR and elemental analyses (Fig. 1). UV-Vis spectra showed that the absorption edge of **P(AQ3)** and **Py-AQ3** was shifted to the longer wavelength region, indicating the expansion of the conjugation length. The electrodes based on **P(AQ3)** and **Py-AQ3** were prepared by mixing with multi-walled carbon nanotubes and graphene. The specific capacity was enhanced to 342 mA h g⁻¹ for **P(AQ3)** and 259 mA h g⁻¹ for **Py-AQ3** at 50 mA g⁻¹ (Fig. 2). *Ex-situ* XAFS analysis indicated the quinone and imine groups act as the reaction sites of Li⁺.

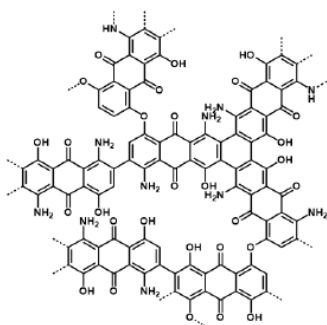


Fig. 1 Estimated structure of **P(AQ3)**.

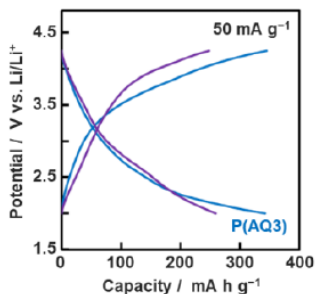


Fig. 2 Charge-discharge curves of **P(AQ3)** and **Py-AQ3**.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Aromatic Diimides: Versatile Building Blocks for Organic Battery Electrode

Materials

Rukiya Matsidik,^{a,b} Konstantin Skudler,^c Sunel de Kock,^d Dipesh A. Sugahiya,^a Milan H. Gotti,^a Mattias Müller,^c Michael Walter,^d Daniele Fazzi^e and Michael Sommer^{a,b}

^a Institut für Chemie, Technische Universität Chemnitz, Straße der Nationen 62, 09111 Chemnitz, Germany

^b Forschungszentrum MAIN, Rosenbergstraße 6, 09126 Chemnitz, Germany

^c Physikalisch-Technische Bundesanstalt, BESSY II, Abbert-Einstein-Straße 15, 12489 Berlin, Germany

^d FIT-Freiburg Center for Interactive Materials and Bioinspired Technologies, University of Freiburg, Georges-Köhler-Allee 105, 79110 Freiburg, Germany

^e Department of Chemistry "Giacomo Ciamician" University of Bologna via P. Gobetti 85, 40129 Bologna, Italy

rukiya.matsidik@chemie.tu-chemnitz.de

michael.sommer@chemie.tu-chemnitz.de

The transition toward renewable energy and the urgent need to electrify all sectors are driving the development of more sustainable, high-performance, and cost-effective energy-storage systems.^[1] Organic electrode materials, constructed primarily from abundant elements (C, H, O, N, S), are emerging as promising alternatives owing to their structural tunability, lower-cost and low-temperature synthesis.^[1,2] Within this material class, aromatic diimides – particularly naphthalene diimide (NDI) – stand out due to their well-defined redox chemistries, structural versatility, and synthetic accessibility.^[3,4]

In this contribution, I will present our recent advances in the design, synthesis and understanding of NDI- and pyromellitic diimide (PMI)- based redox-active polymers for organic battery applications organic, including organic–sulfur and lithium-metal battery systems.^[5–7] Particular emphasis will be placed on how molecular structure, polymer architecture, and redox chemistry influence electrochemical performance. Synthetic strategies, structure–property relationships, redox behavior, and electrode performance of NDI- and PMI-based polymers will be discussed, highlighting the potential of aromatic diimides as versatile building blocks for the development of organic battery electrode materials.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Redox-Active Porous Organic Cage as a Positive-Electrode Material for Rechargeable Lithium Batteries

Ryota Akai, Minami Kato, Saki Fukuma, Masaru Yao

National Institute of Advanced Industrial Science and Technology (AIST)

ryota.akai@aist.go.jp

Organic redox molecules are promising electrode-active materials because they are composed of earth-abundant elements and their electrochemical properties can be tuned through molecular design. However, small-molecule organic redox molecules often suffer from their dissolution in electrolytes, causing the loss of electrode-active material and poor cyclability^[1]. Although increasing molecular weight through polymerization can suppress the dissolution, dense and nonporous polymer structures can hinder electrolyte penetration, thereby restricting ion transport and access to redox-active sites^[2]. In the current work, we investigate a redox-active porous organic cage (RAPOC, Figure a), a discrete molecule with an intrinsic cavity and an intermediate molecular weight^[3]. Its solubility in particular solvents enables detailed structural characterization using solution-based techniques. In addition, its cavity may facilitate electrolyte penetration and ion transport within the bulk electrode. RAPOC demonstrated reversible charge storage in a lithium bis(trifluoromethanesulfonyl)imide (LiTFSI)/diglyme electrolyte (Figure b). In addition, as shown in Figure c, compared with the corresponding small-molecule monomer, the RAPOC exhibited superior cyclability and rate capability. These improvements are attributed to its increased molecular size, which suppresses the dissolution of electrode-active material, and its porous cage architecture, which facilitates efficient mass transport. Therefore, the RAPOC design offers a molecular strategy for addressing two competing challenges in organic electrode-active materials: dissolution-induced cycling instability in small-molecule materials and restricted ion transport in polymeric materials. These findings establish RAPOCs as promising molecular electrode-active materials combining high cyclability and moderate rate capability.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Mediator-Driven Redox Targeting for Polymeric Flow Batteries

Ashley Lam, Samuel Kopfinger, Prof. Shrayesh N. Patel

University of Chicago - Pritzker School of Molecular Engineering

shrayesh@uchicago.edu

Reliable, large-scale energy storage is essential for integrating renewable energy into the grid. Flow batteries are attractive for this purpose because they decouple energy storage from power delivery, but their use has been limited by low energy density. Redox targeting flow batteries offer a promising solution by using solid redox-active materials as the main storage medium (i.e., energy booster), charged/discharged indirectly by soluble mediators.^[1-3] A central challenge is ensuring that this stored capacity is accessible during operation. Our work investigates how mediator choice and design influence capacity utilization of redox-active polymer particles. We study systems with one and two electrochemically active mediators, quantify their ability to access the polymeric particles, and validate a simple thermodynamic model.^[4] These results provide general guidelines for mediator selection and confirm model applicability under practical conditions.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Sustainable 2D Layered Cathode for Alkali-Ion Batteries

Tianyang Chen, Jiande Wang, Bowen, Tan, Mircea Dincă

The Chinese University of Hong Kong (Shenzhen)

chentianyang@cuhk.edu.cn

Eliminating the use of critical metals in cathode materials can accelerate global adoption of rechargeable metal-ion batteries. Organic cathode materials, derived entirely from earth-abundant elements, are in principle ideal alternatives due to their high theoretical specific capacities and practical redox potentials. However, they have not yet challenged inorganic cathodes due to poor conductivity, low practical storage capacity, and poor cyclability. We develop a 2D layered organic cathode material, TAQ, whose high electrical conductivity, high capacity, and complete insolubility enable reversible intercalation/deintercalation of Li^+ , Na^+ , and K^+ ions with small volume change, allowing it to compete at the electrode level with inorganic-based lithium-ion and sodium-ion battery cathodes.^[1-3] It exhibits an electrode-level specific capacity reaching 306 mAh/g and an energy density reaching 765 Wh/kg, as well as an areal capacity reaching 4.5 mAh/cm². The 2D diffusion pathways for alkali-metal ions defined by the hydrogen-bonded molecular layers of TAQ enable high intrinsic rate performance. Engineering of the cathode at composite level, where active material particles are wrapped with carbon nanotubes (only 2 wt.%) through an in-situ growth method, leads to further improvement of rate capability due to enhanced charge transport and transfer kinetics. The electrode exhibits a top energy density over 450 Wh/kg upon a 90-second charging. Furthermore, we demonstrate that TAQ-based lithium battery cells can operate efficiently up to 150 °C. These results demonstrate the operational competitiveness of sustainable organic electrode materials in practical batteries.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Caging polyhalide anions in polycyclodextrin for long-lasting aqueous zinc-iodine batteries

Zhongfan Jia^a

^a Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University, Sturt Road, Bedford Park, SA 5042, Australia

zhongfan.jia@flinders.edu.au

Aqueous zinc-halide batteries have garnered significant attention, but their large-scale deployment is hindered by the migration of polyhalides from the cathode to the zinc anode, which results in severe zinc corrosion and low Coulombic efficiency. Here, we show that poly(β -cyclodextrin) acts as a highly effective and selective host for polyhalide anions, thereby resolving this long-standing shuttling challenge and enabling ultra-long cycling stability.¹ Unlike prior approaches based on nonspecific confinement² or weak ionic interactions,³ our strategy leverages tailored host-guest binding to balance polyhalide retention and release.⁴ By combining experiment and computation, we elucidate the inclusion/release behavior of polyhalides under operating conditions and identify β -cyclodextrin as an optimal host. Crosslinked poly(β -cyclodextrin) gels were synthesized and used to cage KI_3 as the electroactive material. The resulting batteries exhibit stable $2e^-$ and $4e^-$ storage, delivering over 60,000 cycles with capacity retentions of >99% and 85%, respectively, corresponding to exceptionally low capacity losses of 0.0001–0.0003% per cycle. This work establishes a general, molecularly grounded strategy for controlling anion transport and reactivity, with immediate application to improved aqueous zinc-halide batteries and broader implications for host-guest chemistry, catalysis, and functional materials.

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ABSTRACTS OF ORAL CONTRIBUTIONS

Sustainable Quinones at Electrochemical Interfaces: What Can We Learn from Organic Batteries for Adhesives and Carbon Capture?

T. J. Neubert^a, H. G. Börner^b, M. Oschatz^{a,c,d}

^aInstitute for Technical Chemistry and Environmental Chemistry (ITUC), Friedrich Schiller University Jena, 07743 Jena, Germany

^bHumboldt-Universität zu Berlin, Institute of Chemistry, 10117 Berlin, Germany

^cCenter for Energy and Environmental Chemistry Jena (CEEC), Friedrich Schiller University Jena, 07743 Jena, Germany

^dHelmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), 07743 Jena, Germany

tilmann.neubert@uni-jena.de

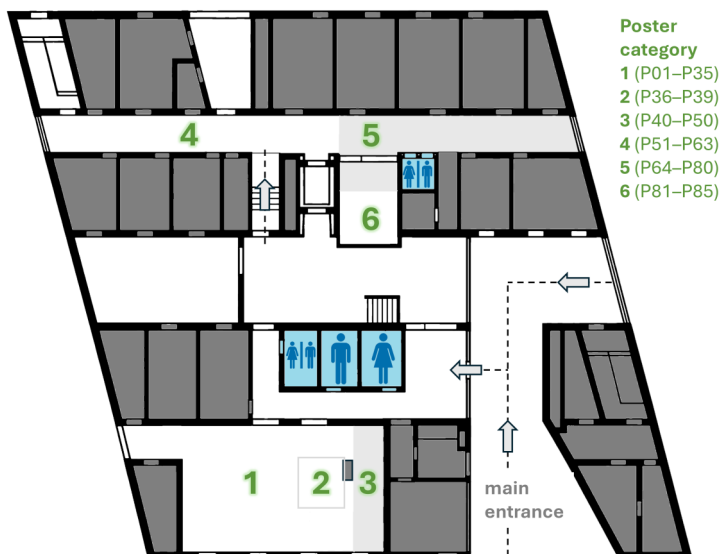
Electrochemical technologies are emerging as important tools for sustainable energy and materials systems. Quinones and related redox-active compounds, abundant in natural resources, are well established as cathode materials in organic batteries and are increasingly being explored for applications such as stimuli-responsive adhesives and electrochemical carbon capture. In adhesive systems, catechols and ortho-quinones govern adhesion and debonding processes. Building on recent advances in polyphenol-based adhesives, we combine lignin-derived catechol-functional polymers with electrochemical cell designs inspired by organic batteries to create structural adhesives that can be selectively deactivated through electrochemical stimulation at the adhesive-adherent interface, enabling on-demand disassembly, repair, and recycling.^[1] In parallel, electrochemical carbon capture based on organic battery components has gained increasing attention due to its high efficiency and tunability. Given the critical importance of carbon management, the use of renewable materials for device fabrication represents a compelling direction.^[2] In this contribution, we demonstrate how quinone-based materials derived from renewable feedstocks can serve as a common electrochemical platform across organic batteries, electrically debondable structural adhesives and electrochemical carbon-capture systems. By exploring shared structure-property relationships governing charge transfer, redox stability and interfacial reactivity, we investigate design principles for multifunctional electroactive materials based on renewable resources.

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Multicomponent covalent organic frameworks with tunable spin states for efficient lithium–carbon dioxide batteries
HIPOLE Jena (DE)
- P 03 Seynabou Diallo
Title to be announced
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P 01: Polymerization of dopamine on graphene oxide for organic active materials of lithium-ion batteries

Fuka Yoshida¹, Yuta Nishina², Yuya Oaki¹

¹Faculty of Science and Technology, Keio University, 3-14-1 Hiyoshi, Kohoku-ku, Yokohama 223-8522, Japan

²Research Institute for Interdisciplinary Science (RIIS), Okayama University, 3-1-1 Tsushimanaka, Kita-ku, Okayama 700-8530, Japan

Introduction Polydopamine (PDPA) is a candidate of organic electrode active materials for lithium-ion batteries. In general, organic active materials have low conductivity. The composites of organic active materials with conductive carbons are required to enhance the specific capacity. As conductive carbons have low capacity, composites with redox-active and conductive materials are required to enhance energy density.¹ In the present study, graphene oxide (GO) which has layered structures, redox-active moieties, and conductivity was used to form the composites with PDPA. The layered composites of dopamine (DPA) and GO were prepared and then the intercalated DPA was polymerized on the layer surface. The PDPA/GO composites were used as both the cathode and anode active materials.

Experimental The DPA-GO composite was obtained by dispersion of GO powder in an aqueous solution containing DPA. DPA was polymerized with addition of ammonia solution to form the PDPA/GO composite. The proportion of PDPA in PDPA/GO was controlled by changing the polymerization time.

Results & Discussion The DPA-GO composite showed the interlayer distance larger than that of GO on the X-ray diffraction (XRD) pattern, indicating the intercalation of DPA into the interlayer space of GO. The weight ratio of DPA in DPA-GO was 13.5 %. The discharge capacity of DPA-GO as a cathode was 157 mA h g⁻¹ at 50 mA g⁻¹. However, the capacity retention rate of DPA-GO was 34 % at 300 cycles because of the dissolution of DPA. The formation of PDPA was analyzed by infrared absorption spectroscopy (IR) and X-ray photoelectron spectroscopy (XPS). The interlayer distance of GO was expanded, and crystallinity was lowered for the PDPA/GO composite. Scanning electron microscope (SEM) images showed that the flat surface of GO was changed to rough after the modification of PDPA (Fig. 1). The PDPA/GO com-

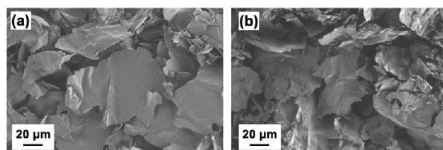


Fig. 1 SEM images of (a) GO and (b) PDPA/GO.

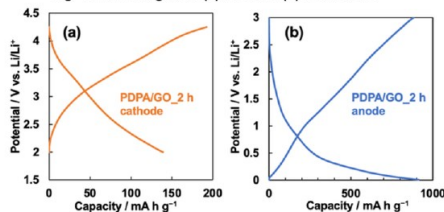


Fig. 2 Charge-discharge curves of PDPA/GO_2 h as cathode (a) and anode (b) active materials.

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posite contained 68.5 wt-% PDPA at the polymerization time for 2 h. The PDPA/GO composite exhibited the highest capacity 133 mA h g^{-1} at 50 mA g^{-1} (Fig. 2a). In contrast, the capacities of PDPA and PDPA/GO mixture were 37 and 67 mA h g^{-1} , respectively. The capacity retention after 300 cycles was improved to 58 %. PDPA/GO showed the discharge capacity 728 mA h g^{-1} at 100 mA g^{-1} as an anode active material (Fig. 2b). Moreover, a full cell using PDPA/GO as both the cathode and anode showed a capacity of 60 mA h g^{-1} . These results indicate that PDPA/GO has potential to use for organic secondary batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 02: Multicomponent covalent organic frameworks with tunable spin states for efficient lithium–carbon dioxide batteries

Jin Yang, Sijia Cao, Yan Lu

HIPOLE Jena, Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

jin.yang@helmholtz-berlin.de

Covalent organic frameworks (COFs) provide a molecular platform for designing structure-defined electrocatalysts, but the synthesis of crystalline low-dimensional COFs with periodically arranged metal sites remains challenging. Here, we report a reticular synthesis strategy for one-dimensional metal COF catalysts toward lithiumsulfur chemistry. The design relies on preorganized metal-chelating building blocks that undergo framework-forming condensation, placing catalytic metal centers directly within an extended covalent scaffold rather than introducing them as external additives.

This contribution focuses on synthetic control over COF dimensionality, crystallinity, and metal-site accessibility. By tuning linker geometry, coordination motif, solvent environment, and condensation conditions, ordered 1D metal COFs with ion-accessible channels and defined local coordination structures are obtained. Powder X-ray diffraction, electron microscopy, gas sorption, X-ray photoelectron spectroscopy, and X-ray absorption spectroscopy are used to correlate synthetic parameters with framework formation and catalytic-site configuration.

As a proof of function, the 1D metal COF is evaluated in lithiumsulfur batteries, where the framework itself serves as a sulfur redox catalyst. Compared with metal-free or non-framework controls, the metal COF promotes polysulfide conversion and lowers electrochemical polarization. This work demonstrates that COF synthesis methodology can be used to program catalytic function into crystalline organic frameworks, offering a general route to low-dimensional, structure-defined electrocatalysts for energy-storage applications.

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P 03: Title to be announced (assigned to "Materials Design & Synthesis")

Seynabou Diallo^{1,2,3}, Sylvestre Toumieux², Matthieu Becuwe^{1,3}

¹Laboratoire de Réactivité et de Chimie des Solides (LRCS), UMR CNRS 7314, Université de Picardie Jules Verne, Hub de l'Energie, 15 rue Baudelocque, Amiens Cedex 80039, France

²Laboratoire de Glycochimie et des Agroressources d'Amiens (LG2A), UR7378, Université de Picardie Jules Verne, 10 rue Baudelocque, Amiens Cedex 80039, France

³Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, Hub de l'Energie, 15 rue Baudelocque, Amiens Cedex 80039, France

seynabou.diallo@u-picardie.fr

A growing interest is being directed towards the field of organic batteries due to its numerous opportunities, especially in reducing the weight, cost, and environmental footprint of energy storage devices. The structural diversity of organic compounds provides significant flexibility, making them especially well-suited for the design of electrode materials and enabling the reduction or even elimination of critical metal use in next-generation batteries.^[1] Among the various classes of organic electrode materials, p-type compounds and especially phenothiazines, undergo reversible oxidation to generate a positively charged state that is compensated by counter anions from the electrolyte, making them well-adapted to anion-storage devices such as Dual-Ion and Anion-Ion batteries.^[2] In this context, our work includes the synthesis of a series of nonpolymeric phenothiazine materials exhibiting redox potentials equal to or exceeding 3.6 V vs. Lithium. The dimerization strategy of phenothiazine has been shown to offer superior capacity retention and electrochemical performance, with specific capacities approaching the theoretical value.^[3] Therefore, our study focuses on the molecular design, with the aim of investigating how structural and chemical modifications influence the resulting redox potentials and overall electrochemical behaviour. The investigation comprises the synthesis of the target compounds via efficient coupling reactions, their physicochemical characterization, and the evaluation of their electrochemical performance in lithium half-cells (dual-ion configuration), with a view to their application as positive electrode materials in organic batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 04: Emerging of room-temperature spin coherence in semiconductive two-dimensional poly(arylene vinylene)s

Yamei Liu

Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

yamei.liu@mpi-halle.mpg.de

High-performance battery electrodes require the coordinated optimization of redox chemistry, electronic charge transport, and mass transport. Two-dimensional conjugated polymers and covalent organic frameworks (2D c-COFs), with molecularly tunable π -conjugated backbones and well-defined porous architectures, provide a versatile platform for addressing these requirements. Our studies establish complementary molecular and structural strategies for regulating transport in 2D conjugated frameworks. Incorporating planar thiophene-rich backbones enhances π -delocalization and enables band-like charge transport, with room-temperature carrier mobilities reaching $\sim 65 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [1]. At a larger structural scale, ordered bicontinuous mesochannels improve mass transport and access to internal active sites [2]. In contrast, intralayer structural anisotropy offers an additional degree of freedom for directing charge transport. These concepts are directly relevant to electrochemical energy storage. Electron-deficient 2D PAVs effectively confine sulfur/polysulfide species and facilitate host-guest charge transfer. Sulfur-loaded 2D PAV cathodes deliver a specific capacity of 1086 mAh g^{-1} at 0.1 C and retain 80.1% of their capacity after 200 cycles in LiS batteries [3]. We further reveal that progressive oxidation of fully conjugated 2D PAVs generates delocalized radical/polaronic states and strongly regulates charge-carrier dynamics. The carrier scattering time increases from 10.6 to 54.8 fs, accompanied by a mobility enhancement from approximately 30 to $156 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. These results demonstrate a multiscale electrode-design strategy that integrates π -conjugation, electron affinity, pore architecture, and redox-state-dependent charge delocalization for next-generation rechargeable batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 05: Bridging energy and power density gap: Multi-redox CMP/CNT composite as high loading organic cathode for lithium-ion battery

Gulraiz Tanvir

Beijing Institute of Technology, China

Conjugated microporous polymers (CMPs) are emerging as promising organic cathode materials for lithium-ion batteries due to their high surface area, structural tunability, and fast redox kinetics. Practical implementation remains limited by low intrinsic conductivity, incomplete active material utilization, and cycling degradation. A phenazine-based conjugated microporous polymer (TPA - DPZ CMP) was synthesized via Buchwald–Hartwig coupling and integrated with acidfunctionalized carbon nanotubes (CNTs) through in-situ polymerization to form a conductive composite (TPA-DPZ@CNT). The polymer design combines triphenylamine (TPA) and dihydrophenazine (DPZ) redox units, which are known high-potential cathode motifs but suffer from dissolution and instability in their molecular form. Incorporation into a CMP architecture suppresses dissolution but results in limited conductivity and sluggish charge transport. To overcome these limitations, acid-functionalized CNTs were introduced to create non-covalent interactions between the polymer framework and the CNT surface, generating a robust interconnected conductive network.

The resulting composite exhibits significantly enhanced electrical conductivity, faster ion diffusion, and improved charge-transfer kinetics compared with the pristine CMP. Consequently, the cathode demonstrates exceptional rate capability, retaining 53% capacity at an ultrahigh current density of 20 A g^{-1} ($\approx 266\text{C}$), corresponding to a full charge within 13 s. Notably, this high-rate performance is achieved with a high active material content (80%) and areal loading of $1.5\text{--}2 \text{ mg cm}^{-2}$. Increasing the active material content to 90% still delivers a high capacity of 118 mAh g^{-1} at 1 A g^{-1} while maintaining excellent rate performance. Density functional theory calculations indicate a reduced bandgap in the polymer relative to the individual monomers, supporting improved electronic transport across the extended conjugated structure. The optimized composite (TPA- DPZ@CNT 5%) also shows remarkable cycling stability, retaining 83 mAh g^{-1} over 10,000 cycles at 1 A g^{-1} . The electrode delivers a high energy density of 445 Wh kg^{-1} together with a power density of 67 kW kg^{-1} , bridging the typical performance gap between lithium-ion batteries and ultracapacitors. Full-cell evaluation further confirms competitive initial capacity and excellent rate capability compared with commercial cathodes. These results demonstrate that constructing conductive polymer–CNT networks provides an effective strategy for maximizing active material utilization and enabling high-power, long-life organic cathodes for next-generation energy storage.

ABSTRACTS OF POSTER PRESENTATIONS

P 06: Modification and characterisation of ketazines as anolytes for two-electron storage in non-aqueous flow batteries

Caroline Witter^{1,2}, Karin Sowa³, Robert Hein², Mariano Grünebaum¹

¹Forschungszentrum Jülich GmbH, Helmholtz Institute Münster, 48149 Münster, Germany

²University of Münster, Institute of Organic Chemistry, 48149 Münster, Germany

³University of Münster, MEET Battery Research Center, 48149 Münster, Germany

cwitter@uni-muenster.de

Redox flow batteries (RFBs) are promising technologies for large-scale and long-duration grid energy storage as they can decouple power and energy capacity.^[1] However, aqueous RFBs are limited by the relatively narrow electrochemical stability window of water, which restricts the achievable cell voltage. Non-aqueous electrolytes offer a wider electrochemical window, enabling higher cell voltages. Molecular design strategies for organic redox active materials have therefore focused on optimizing redox potentials, stability, solubility and cost, while also introducing multi-electron redox processes.^[1] Ketazines represent promising anolyte materials for non-aqueous RFBs due to their ability to undergo a simultaneous two-electron transfer at reducing potentials around -1.02 V vs Fc/Fc⁺.^[2] Building on previously investigated systems, molecular engineering was employed to tune the reduction potential as low as -1.14 V. This translates to an approximately 9% increase in cell voltage while maintaining comparable cycling stability. In addition, the investigated ketazines exhibit a solubility of up to 0.7 M in acetonitrile. These properties highlight the potential of molecularly engineered ketazines as high-energy-density anolytes for non-aqueous flow battery applications.

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P 07: Electrode materials via electropolymerization of stable organic radicals

Christian Friebe¹, Clara Zens², Stephan Kupfer², Ulrich S. Schubert^{1,3}

¹Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

²Institute for Physical Chemistry (IPC), Friedrich Schiller University Jena, Helmholtzweg 4, 07743 Jena, Germany

³Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

christian.friebe@helmholtz-berlin.de

Today's battery technologies are based primarily on metals, such as lithium, lead, cobalt, and nickel. However, their limited natural reserves, as well as their toxicity and the resulting disposal problems, limit the future use of such metals^[1]. In this context, polymer compounds containing stable organic radicals have emerged as an alternative and have been studied extensively. They demonstrated advantageous charge-storage properties, in particular superior redox kinetics, but suffer from insufficient electrical conductivity, which limits the applicable charging and discharging rates^[2]. A promising approach to overcoming this problem is the incorporation of conductive, i.e., conjugated polymers. These combined materials offer several beneficial properties that can be exploited for an organic battery: (i) they exhibit electrical conductivity; (ii) they can be produced by electropolymerization, thus providing an efficient means of depositing them directly onto electrode surfaces; (iii) they possess intrinsic charge storage capacity. This study aims at the development of suitable polymeric systems, which contain stable organic radical moieties for charge storage and can be obtained via electropolymerization, within a joined experimental-computational approach. While the experimental work focuses on the preparation of modular building blocks that contain stable organic radicals as well as electropolymerizable units, theoretical computations assess the redox as well as charge-transfer properties to identify suitable candidate molecules. Hence, a promising system was found, namely a combination of (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) and terthiophene, demonstrating the charge-storage ability of an electrochemically prepared polymer film^[3]. Further investigations focus on the tackling of identified challenges, e.g., long-term stability and charge-transfer capability.

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ABSTRACTS OF POSTER PRESENTATIONS

P 08: Methylphenoxazine-based polymer as cathode-active material for organic-aluminum batteries

Eva Bräutigam, Birgit Esser*

Institute of Organic Chemistry II and Advanced Materials, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

CELEST Green Energy Lab Ulm

eva.braeutigam@uni-ulm.de

With aluminum being the most abundant metal in the Earth's crust, rechargeable aluminum batteries (RABs) are promising candidates for next-generation energy storage.^[1] However, the development of suitable positive electrode materials remains a major challenge. Previous work by Studer et al. demonstrated the excellent performance of the crosslinked methylphenothiazine-based polymer (X-PVMPT), delivering specific capacities of up to 167 mA h g⁻¹ and retaining 88% of its capacity after 5000 cycles at 10C.^[2] Building on these results and our previous investigation of X-PVMPO vs Li | Li⁺, which revealed an enhanced rate capability compared to X-PVMPT,^[3] we herein investigate a related cross-linked polymer containing methylphenoxazine units (X-PVMPO) as a positive electrode material for RABs. In addition to its electrochemical performance, we investigate the underlying redox and charge-storage mechanisms, with particular focus on the interaction of the MPO redox centers with the chloroaluminate electrolyte and the influence on electrochemical cycling.

The results provide insights into the relationship between polymer structure, redox activity, and electrolyte interactions, highlighting crosslinked methylphenoxazine-based polymers as positive electrode materials for RABs employing ionic liquid electrolytes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 09: Triphenylamine-based polymer cathodes for lithium and sodium batteries: Influence of network density and ionic functionality

Eva Van Doeselar¹, Janine Richter², Eric McCalla², Klaus Meerholz^{1*}

¹University of Cologne, Department of Chemistry and Biochemistry, Institute of Light and Matter

²McGill University Montréal, Department of Chemistry

e.vandoeselar@uni-koeln.de

Triphenylamine-based p-type cathodes enable reversible charge storage in both lithium- and sodium-based battery systems. High operating voltages of around 3.5 V vs. Li/Li⁺ and 3.3 V vs. Na/Na⁺ together with high rate capability and cycling stability, are achieved through the formation of an insoluble polymer network via in situ cationic ringopening polymerization (CROP) of oxetane-functionalized TPA cores ^[1]. By varying the number of oxetane functionalities (one vs. two) on the TPA core, the network density of the cathode was tuned. Despite this structural variation, electrochemical utilization remains largely unaffected in both lithium and sodium-based systems. PITT -derived diffusion coefficients are of similar magnitude ($1-3 \times 10^{-10}$ cm²/s), indicating little influence of crosslinking density on ion transport, if at all. Within the oxetane-functionalized TPAs, the di-oxetane derivative reaches utilization values of 89% at 1C in Li-based cells and 81% in Na-based cells. To modulate the charge compensation behavior, SO₃M-functionalized additives or structural variations to the TPA-based cathode introduce alkali ion charge balancing, thereby reducing the contribution of electrolyte anion. This concept is referred to as balanced ion movement, in which both cation and anion migration contribute to electroneutrality at the cathode. Notably, lithium-based additives enable ultrahigh rate capability up to 400 C while PITT -derived diffusion coefficients remain comparable to those of the pristine system. Overall, the results demonstrate that TPA-based cathodes are suitable as high-voltage cathode materials for both lithium- and sodium-based systems. The ionic functionality can influence the balance between dual-ion and rocking-chair-like charge storage mechanism.

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ABSTRACTS OF POSTER PRESENTATIONS

P 10: Synthesis and electrochemical investigation of anthraquinone-based redox monomers for electrochemical CO₂ capture

Fabian Knötzsch^{1,2}, Stefan Zechel¹⁻⁴, Martin D. Hager¹⁻⁵, Tilmann Joachim Neubert⁶, Hatice Mutlu¹⁻³, Ulrich S. Schubert¹⁻⁵

¹Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

²Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

³Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, 07743 Jena, Germany

⁴Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Philosophenweg 7, 07743 Jena, Germany

⁵Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

⁶Institute for Technical and Environmental Chemistry (ITUC), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

fabian.knoetzschi@helmholtz-berlin.de

Electrochemical CO₂ capture is a promising approach for developing more energy-efficient alternatives to conventional capture methods.^[1] A key concept involves the use of redox-active organic materials whose affinity for CO₂ can be reversibly switched by applying an electric potential. Quinones are particularly interesting for this purpose, as their reduction leads to nucleophilic species that can interact reversibly with CO₂.^[1,2] Anthraquinones are in particular well-suited as molecular building blocks due to their well-established redox chemistry and the ability to introduce various functional groups, e.g., polymerizable groups, without altering the quinone core.^[3]

In this work, we developed a systematic library of six polymerizable anthraquinone monomers to investigate how the different linker structures affect their electrochemical behavior and the interaction with CO₂. The resulting monomers were characterized using ¹H and ¹³C NMR spectroscopy, GC-MS, ESI-TOF, elemental analysis, UV/VIS spectroscopy, and cyclic voltammetry under air, nitrogen, and CO₂ atmospheres. By systematically varying the molecular structure while keeping the anthraquinone unit constant, we aim to identify structure-property relationships that can be used to specifically control the redox behavior and CO₂ responsiveness of anthraquinone-based materials. These findings form the first basis for the subsequent development of redox-active polymer systems for electrochemical CO₂ capture.

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ABSTRACTS OF POSTER PRESENTATIONS

P 11: Development of p-type organic electrode materials for anion-ion batteries

Florian Livernaux^a, Lionel Dubois^b, Thibaut Gutel^a

^aUniv. Grenoble Alpes, CEA, Liten, DEHT, F-38054 Grenoble, France

^bUniv. Grenoble Alpes, CEA, CNRS, Grenoble INP, IRIG, SyMMES, F-38054 Grenoble, France

florian.livernaux@cea.fr

Although lithium-ion batteries currently dominate the energy storage market, alternative technologies are needed due to the limited availability of critical raw materials, toxicity concerns, and the high energy demand of their production. Organic electroactive materials (OEMs) are promising candidates for next-generation energy storage systems because they reduce reliance on critical raw materials and lower the environmental footprint of their production.^[1] Among the opportunities offered by OEMs, the anion-rocking-chair configuration is promising due to the higher molar conductivity of anions in conventional electrolytes and the absence of metallic charge carriers, improving battery safety while reducing reliance on critical raw materials.^[2] However, the lack of p-type redox-active materials with low redox potentials remains a major challenge, limiting the cell voltage. Among the reported compounds, bipyridinium salts, also known as viologens, are the most promising, exhibiting relatively low redox potentials (2.0–2.5 V vs Li⁺/Li). However, these values remain too high to reach high cell voltage. Previous studies have shown that introducing an aromatic linker between the two pyridinium units brings the redox processes closer together in potential, while also lowering the overall redox potential.^[3] In this work, we report the synthesis and electrochemical characterization of a library of molecular π -extended viologens, including a comparative study of different linkers by electrochemical characterization in both solution and solid-state, in order to identify the best strategy to reduce the redox potentials of this type of compounds. This work provides new insights into the development of new negative electrodes for high energy density battery in anion-ion configuration.

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ABSTRACTS OF POSTER PRESENTATIONS

P 12: Organic electrode materials for resource-abundant Mg and Ca battery systems

Hikaru Sano¹, Minami Kato¹, Yuta Doki², Kazuaki Kisu², Saki Fukuma¹, Naoya Ishida¹, Keigo Kubota¹, Masaru Yao¹

¹National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577, Japan

²College of Engineering, Shibaura Institute of Technology, 3-7-5 Toyosu, Koto-ku, Tokyo 135-8548, Japan

hikaru.sano@aist.go.jp

Organic electrode materials are promising cathode candidates for resource-sustainable rechargeable batteries because they can reduce reliance on transition-metal-based inorganic cathodes. Replacing Li^+ with more abundant carrier ions such as Mg^{2+} and Ca^{2+} is also attractive for further cost reduction.^[1] However, these divalent ions interact strongly with counter anions, solvents, and electrode materials, making reversible battery operation difficult. Recent electrolytes designed to weaken cation-solvent and cation-anion interactions have opened opportunities for Mg and Ca batteries,^[2,3] but cathode reactions remain a key challenge. Organic active materials are attractive because their flexible molecular structures may accommodate strongly interacting multivalent ions more readily than rigid inorganic frameworks. Here, we investigated organic cathode materials in Mg- and Ca-based battery systems. For the Ca-based system, a cell was assembled using a Ca metal anode, a 2,5-dimethoxy-1,4-benzoquinone (DMBQ) composite cathode, and $\text{Ca}[\text{CB11H12}]_2$ in a DME/THF mixed solvent. Clear charge-discharge plateaus were observed, suggesting that the two-phase redox reaction of DMBQ proceeded in the Ca electrolyte (Figure). Energy-dispersive X-ray spectroscopy (EDS) after charge and discharge revealed reversible changes in the Ca/F elemental ratio, where F from the PTFE binder was used as an internal reference, providing evidence for Ca insertion and extraction during cycling (Figure). Detailed experimental results for both Mg- and Ca-based systems will be presented, highlighting the potential of organic electrodes for low-cost, resource-abundant post-Li battery technologies.

ABSTRACTS OF POSTER PRESENTATIONS

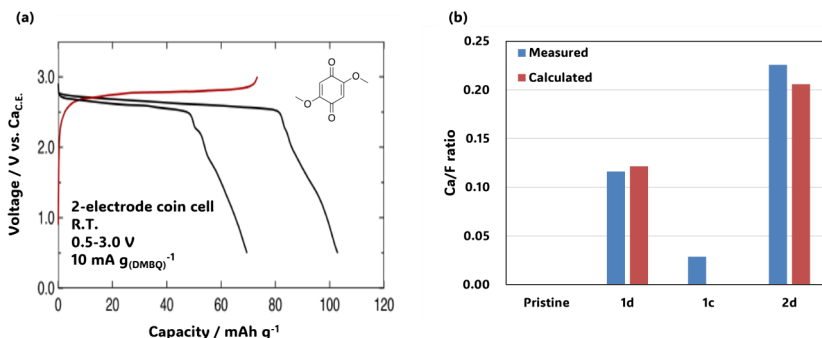


Figure. (a) Charge–discharge profiles of a DMBQ composite cathode with a Ca metal anode and $\text{Ca}[\text{CB}_{11}\text{H}_{12}]_2$ in DME/THF electrolyte. (b) Ca/F atomic ratios of the DMBQ composite cathode after discharge and charge. The measured values were determined by EDS using F from the PTFE binder as an internal reference, and the calculated values were estimated from the capacities in the charge–discharge profiles.

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ABSTRACTS OF POSTER PRESENTATIONS

P 13: Geometry-driven state-selective redox potential tuning to achieve multi-redox in phenoxazine-based organic cathodes

Joohwan Eo^{1,2}, Sunwo Song¹, Dong Hyeon Jo^{1,2}, Min Sang Kwon^{1*}, Ji Eon Kwon^{2,3*}

¹Department of Material Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul 08826, Republic of Korea

²Jeonbuk Institute of Advanced Composite Materials, Korea Institute of Science and Technology (KIST), 92 Chudong-ro, Bongdong-eup, Wanju-gun, Jeonbuk 55324, Republic of Korea

³Department of JBNU-KIST Industry Academia Convergence Research, Jeonbuk National University, 567 Baekje-daero, Deokjin-gu, Jeonju-si, Jeonbuk 54869, Republic of Korea

jekwon@kist.re.kr

Organic p-type cathodes offer high operating voltages but often suffer from low capacity utilization due to inaccessibly high redox states beyond the electrochemical stability window of conventional electrolytes^[1]. Here, we introduce a molecular design strategy, state-selective redox potential tuning (SSRPT), that selectively modulates the energetics of only a targeted redox state through oxidation-induced geometric and electronic reorganization of peripheral substituents. By activating decoupled -conjugation between the redox core and substituents upon oxidation, SSRPT lowers the second oxidation potential of the redox core without substantially altering its first redox potential. To demonstrate this concept, a phenoxazine (PXZ) redox core capable of undergoing two sequential single-electron oxidations is functionalized by four electron-donating substituents, including methoxy (MeO), diphenylamine (DPA), carbazole (Cz), and phenoxazine (PXZ). Whereas MeO and DPA lower both redox potentials, Cz and PXZ selectively decrease the second oxidation potential of the PXZ core by 540 and 620 mV, respectively, without substantially shifting the first oxidation potential. In particular, Cz-substituted PXZ (Cz-PXZ) enables a reversible multi-electron redox process within the electrolyte stability window, delivering a high average operating voltage of 3.92 V vs. Li/Li in a Li-organic cell. Furthermore, oxidative coupling between Cz units induces in situ electrochemical crosslinking during cycling, suppressing dissolution and substantially improving cycling stability.

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ABSTRACTS OF POSTER PRESENTATIONS

P 14: Redox behavior of azo-functional covalent organic framework cathodes for lithium-metal batteries

Kamaldeep Kumar, Rebeca Marcilla, Vikram Singh

IMDEA Energy Institute, Madrid, Spain

vikram.singh@energia.imdea.org

Covalent organic frameworks (COFs) are promising electrode materials for organic batteries owing to their structural modularity, incorporation of redox-active organic units, and well-defined ion-transport pathway.^[1,2] However, establishing relationships among molecular-level redox processes, framework structure, and electrochemical response remains challenging.^[1] In this context, azo functionalities provide an attractive redox-active motif for Li storage, while their molecular level electrochemical behavior within COF architecture remains insufficiently understood^[3]. Here, we investigate two azo-functional COFs as cathodes in lithium-metal batteries through complementary electrochemical, ex situ, morphological, and operando characterization. Two azo-functional COFs were synthesized as redox-active cathode for lithium-metal batteries. The frameworks differ in hydroxy functionality, molecular symmetry, and solvent-dependent structural organization, resulting in distinct crystallographic, morphological, and electrochemical characteristics. Electrochemical measurements reveal different redox behaviors and lithium-storage properties, while operando Raman and infrared spectroscopy track the evolution of azorelated vibrational features during lithiation and delithiation. Operando X-ray diffraction further reveals changes in crystallinity and structural response during cycling. Together, these results establish relationships among molecular functionality, framework structure, and lithium-storage chemistry and highlight the role of hydroxy groups, molecular symmetry, and synthesis solvent in governing redox behavior and framework crystallinity.

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ABSTRACTS OF POSTER PRESENTATIONS

P 15: Glutamic acid–functionalized naphthalene diimide as a highly soluble anolyte for aqueous organic redox flow batteries

Kimia Hoseinzade, Rene Wilhelm

TU Clausthal

kimia.hoseinzade@tu-clausthal.de

Naphthalene diimide (NDI) derivatives show great potential as redox-active materials for aqueous organic redox flow batteries (RFBs). (Wang et al., 2024) They are known for their two-electron storage capability, and the π conjugation across the aromatic core stabilizes the molecular structure. (Shahsavan et al., 2026) However, strong π - π interactions have traditionally limited their application to non-aqueous systems or solid-state electrodes. To enable the use of NDIs in aqueous RFBs, solubility and self-association behavior can be tuned through appropriate side-chain and functional-group modification at the imide positions. Building on our previous work on aqueous organic redox-active materials for RFBs (Caianiello et al., 2023), in this work, we present a new anionic glutamic acid -functionalized naphthalene diimide (Glu-NDI, Et_3NH^+ salt), designed to achieve enhanced aqueous solubility and improved electrochemical performance. The new molecule was comprehensively characterized using electrochemical and chemical methods. Furthermore, a laboratory-scale full-cell flow battery demonstration is reported, employing Glu-NDI as the negolyte and the well-known $\text{K}_4[\text{Fe}(\text{CN})_6]/\text{K}_3[\text{Fe}(\text{CN})_6]$ redox couple as the posolyte. During extended cycling, the ferrocyanide-based posolyte gradually degraded to a Prussian Blue -type solid that deposited on the membrane and flow tubing, confirmed by FTIR against a commercial Prussian Blue reference. This represents an independent degradation pathway for near-neutral ferrocyanide posolytes, which a simple cyanide-based pretreatment of the positive electrode was found to substantially suppress, extending the full cell's practical cycle life.

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ABSTRACTS OF POSTER PRESENTATIONS

P 16: Synthesis of trifurcated viologen-substituted polymer with inhibited redox-induced viscosity change

Kohei Ishigami, Hana Sato, Kisho Hiruba, Shinjiro Mori, Kenichi Oyaizu

Department of Applied Chemistry, Waseda University

oyaizu@waseda.jp

Redox-active polymers are promising for energy storage applications such as aqueous organic redox flow batteries, as they allow for the tuning of resource supply stability, electrochemical stability, and physical properties. One significant advantage from the perspective of PFAS regulations is the ability to replace fluorine-containing ion-exchange membranes with nanoporous membranes.^[1] To ensure water solubility, conventional development has heavily relied on copolymerization; however, this approach suffers from an exponential increase in viscosity at higher concentrations, limiting the theoretical capacity to approximately 10 Ah/L. To overcome this limitation, redox-active polyelectrolytes with a high ionic density per monomer unit have recently been proposed, enabling low viscosity and high fluidity even at capacities exceeding 20 Ah/L—a performance level previously unattainable. While introducing branched structures into redox-active polymers has been reported as an approach to reduce electrolyte viscosity,^[3] studies that systematically elucidate viscosity changes as a function of the state of charge (SoC) remain rare.

In this study, we report the synthesis of a trifurcated, low-viscosity viologen-substituted polymer via precise radical polymerization and post-functionalization. Viologen was selected for its highly reversible redox response in pH-neutral aqueous electrolytes. The electrolytes containing this trifurcated polymer successfully exhibited reduced dynamic viscosity and significantly suppressed viscosity changes upon redox compared to their linear polymer.

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ABSTRACTS OF POSTER PRESENTATIONS

P 17: High-performance organic cathode and electrolyte for sodium metal batteries

Litwin Jacob^{a,b}, Chinmaya Mirle Ramachandra^{a,b}, Philipp A. Schuster^a, Luis Kolb^a, Ziyuan Lyu^{b,c,d}, Dominic Bresser^{b,c,d,e}, Alexander J.C. Kuehne^{a,b}

^aUlm University, Institute of Organic and Macromolecular Chemistry, 89081 Ulm, Germany

^bCELEST Green Energy Lab Ulm, Ulm University, Lise-Meitner-Str. 16, 89081 Ulm, Germany

^cHelmholtz Institute Ulm for Electrochemical Energy Storage (HIU), 89081 Ulm, Germany

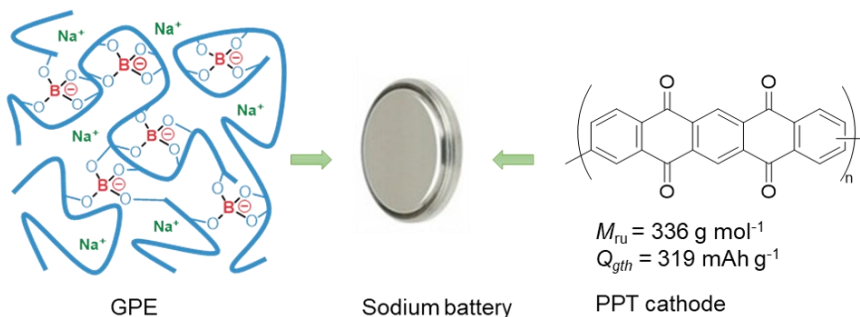
^dKarlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

^eUlm University, 89069 Ulm, Germany

litwin.jacob@uni-ulm.de; alexander.kuehne@uni-ulm.de

The surge in energy demand and the quest for sustainability position organic batteries as potential alternatives to conventional inorganic systems. Particularly interesting among them are the rechargeable sodium metal batteries (SMBs), which represent promising alternatives to lithium batteries (LBs) because of the high natural abundance of sodium, prospectively low production costs, and identical internal components and charge-discharge principles compared to LBs.^[1] Cathodes and electrolytes are key components for batteries, and they critically influence the specific capacity, cycling performance, working temperature range, and safety of batteries. Redox-active organic compounds, particularly π -conjugated quinones, have emerged as a viable alternative to conventional inorganic cathodes due to their tunable electrochemical properties, structural flexibility, and enhanced compatibility with Na-metal.^[2] Despite their advantages, many quinone-based cathodes suffer from limited cycling stability and solubility issues. Recent studies have shown good compatibility of ether-based electrolytes with sodium metal anodes. However, the commercial application of conventional liquid electrolyte-based SMBs is still challenging due to serious safety hazards, including high volatility, inflammability and leakage, severe side reactions between electrodes and electrolytes, and inevitable problems of sodium dendrite formation.^[3] In this context, I will present our investigation on poly(pentacenetetrone) (PPT) as a high-capacity cathode and a fluoropolymer-based gel polymer electrolyte (GPE) crosslinked by NaBH₄ as solutions to the critical problems of organic cathode and electrolyte described above. The ionic conductivity, transference number studies of the gel electrolyte, electrochemical characterization, and battery cycling performance of the gel and the PPT cathode material will be discussed.

ABSTRACTS OF POSTER PRESENTATIONS



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ABSTRACTS OF POSTER PRESENTATIONS

P 18: Polyphosphazene-based cathodes for IoT-oriented organic batteries

Lucas Marquart, Martin Winter, Gunther Brunklaus

Forschungszentrum Jülich GmbH, Helmholtz-Institut Münster (IMD-4), NRW, Germany

l.marquart@fz-juelich.de

The expanding markets for wearable technology and other Internet of Things (IoT) applications are fueling a demand for efficient and safe batteries.^[1] Unlike conventional battery materials, which are based on transition metals, organic battery active materials are derived from carbon-based resources. Consequently, they represent not a replacement, but rather a complementary addition to the field of inorganic active-material-based batteries.^[2] However, as of yet, their application readiness faces challenges. Their synthesis is often more complex compared to inorganic materials and the materials themselves present drawbacks such as electrolyte solubility, insufficient conductivity and lower half-cell potentials. In view of favorite features, they often afford fast charging, which is an advantage in many applications. Poly(2,2,6,6-tetramethyl-1-piperidinyloxy-4-yl methacrylate) (PTMA) represents a valid reference for organic battery cathode materials due to its vastly explored, highly optimized structure and its fast and reliable cycling performance driven by its persistent radical moiety but also its straight-forward synthesis approach ($C_{theo} = 111 \text{ mAh g}^{-1}$).^[2] Based on that, TEMPO-grafted (poly)-phosphazenes (TG PPZ) were developed as derivatives of PTMA, addressing key challenges such as low ion diffusivity that is linked to the rigid polymer backbone MMA compared to PPZ. ^[3] TG-PPZ ($C_{theo} = 132 \text{ mAh g}^{-1}$) offers a higher theoretical specific capacity compared to PTMA due to double functionalization. The materials demonstrated initial specific discharge capacities of up to 56.5 mAh g^{-1} at rates of up to 1C (0.1 mAh). To align expected and experimentally measured capacities, multiple TG-PPZ polymers with variable degrees of cross-linking were prepared, thereby analyzing differences introduced by cross-linking density upon cycling and rate capabilities.

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ABSTRACTS OF POSTER PRESENTATIONS

P 19: Super-electron-donor polymers: From monomer design to redox functionality

Luisa Rzesny^{1,2}, Aswadh Shyma Sajeevan³, Caroline Schmidt⁴, Johannes Lahr⁴, Christoph Lorenz¹, Mathias Hermann¹, Nicolas Dupré³, Stéven Renault³, Philippe Poizot^{3*}, Birgit Esser^{1,2*}

¹Institute of Organic Chemistry II and Advanced Materials, Ulm University, Ulm, Germany

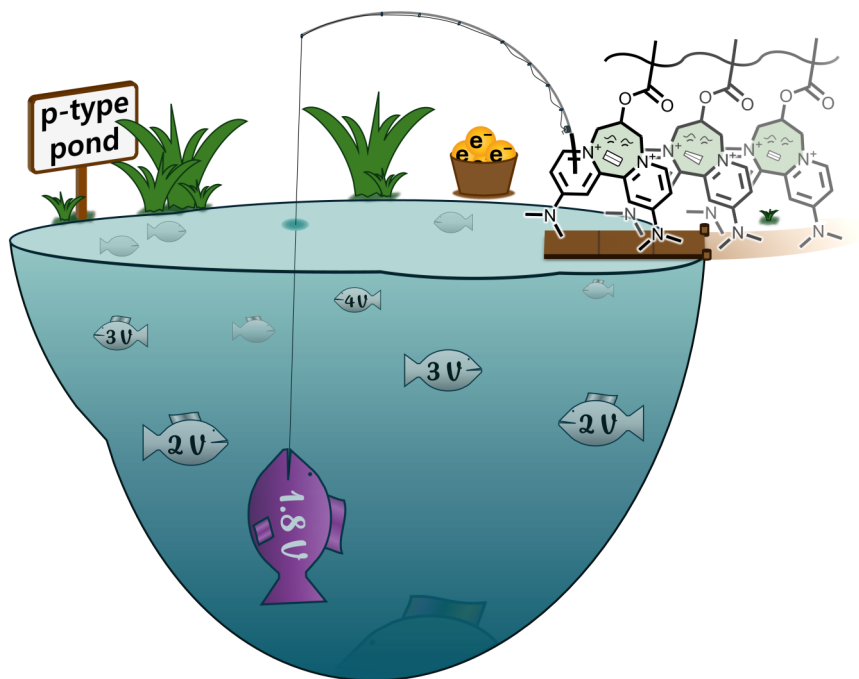
²CELEST Green Energy Lab Ulm, Ulm University, Ulm, Germany

³Nantes Université, CNRS, Institut des Matériaux de Nantes Jean Rouxel, IMN, Nantes, France

⁴Institute of Organic Chemistry, University of Freiburg, Freiburg im Breisgau, Germany

luisa.rzesny@uni-ulm.de

Organic electrode-active materials are contributing to an increasing variety of energy storage systems. However, there are only a few examples of p-type materials with low redox potential (< 2 V vs. Li/Li⁺) which are particularly relevant for the negative electrode of anionic-rocking chair full cells.^[1] In this cell configuration, charges are balanced exclusively by anions from the electrolyte, allowing the battery to function without metal cations.^[2] 2,2'-Bipyridinylidenes are known for their super-electron-donor (SED) properties and have therefore been used beyond the field of organic synthesis. Their two-electron redox process at low potential makes them attractive p-type materials for the negative electrode.^[1] Here, we present a synthetic approach in which hydroxy-functionalized, bridged 2,2'-bipyridinium units (as the stable, oxidized form of SEDs) are incorporated into a polymer. In this modular synthesis the redox unit is attached to an aliphatic backbone, ensuring a stable redox potential. The resulting reduced solubility allowed for an initial electrochemical evaluation of the polymer in a lithium-organic half-cell, where we observed a low redox potential of 1.8 V vs. Li/Li⁺. We demonstrate that this novel class of SED polymers has the potential to serve as active material in organic electrodes.^[1]



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ABSTRACTS OF POSTER PRESENTATIONS

P 20: Spatial confinement of self-adsorbed pillar[5]quinone in porous carbon hybrid for sodium-organic batteries

Mengyu Chen^a, Yannik Hansmann^b, Birgit Esser^{b,c,d}, Tilmann J. Neubert^a, Martin Oschatz^{a,e,f}

^aFriedrich Schiller University Jena, Institute for Technical Chemistry and Environmental Chemistry (ITUC), 07743 Jena, Germany

^bUlm University, Institute of Organic Chemistry II and Advanced Materials, 89081 Ulm, Germany

^cUlm University, CELEST Green Energy Lab Ulm, 89081 Ulm, Germany

^dHelmholtz Institute Ulm (HIU), Electrochemical Energy Storage, 89081 Ulm, Germany

^eFriedrich Schiller University Jena, Center for Energy and Environmental Chemistry Jena (CEEC), 07743 Jena, Germany

^fHelmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), 07743 Jena, Germany

mengyu.chen@uni-jena.de

Organic batteries have emerged as one of the most attractive candidates for sustainable energy storage devices owing to their composition of earth-abundant elements (C, H, and O) and chemical tunability, which enables high theoretical capacities. However, the practical application of organic batteries is limited due to the inherent poor electrical conductivity and high solubility of organic electrode materials in commercial electrolytes. To address this challenge, organic molecules with a high electron-storage capacity can be combined with conductive carbon materials with a high specific surface area to combine their favourable properties. Herein, a zinc oxide templated carbon (ZTC) is impregnated with pillar[5]quinone (P5Q) ^[1] to form hybrid materials (P5Q@ZTC). P5Q self-adsorbs from a solution onto the surface of ZTC, whereby it is immobilized through spatial confinement on the nanoscale. P5Q serves as the redox-active component for energy storage, while ZTC forms a matrix for P5Q, providing abundant adsorption sites to significantly mitigate the dissolution of P5Q. Simultaneously, ZTC is forming an interconnected conductive framework to overcome the challenge of slow reaction kinetics in sodium-organic batteries. The ratio of ZTC to P5Q was systematically varied during the self-adsorption process to identify an optimal balance between active material loading and electrochemical accessibility. At optimized conditions, a reversible capacity of approximately 400 mAh g⁻¹(P5Q) at 0.05C was retained over more than 70 cycles, indicating efficient stabilization and utilization of the redox-active P5Q within the conductive carbon matrix. This study demonstrates that active material utilization and capacity retention are strongly governed by the interplay between nanoscale confinement, electronic connectivity, and electro-

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lyte accessibility.

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ABSTRACTS OF POSTER PRESENTATIONS

P 21: Dihydrophenazine-based nanohoops as organic electrode active material

Michael Keis, Birgit Esser*

Institute of Organic Chemistry II and Advanced Materials, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

CELEST Green Energy Lab Ulm, Ulm University, Lise-Meitner-Str. 16, 89081 Ulm, Germany

michael.keis@uni-ulm.de

While macrocycles have already been used occasionally as organic battery electrode active materials, conjugated nanohoops with defined redox-active groups (RAGs) have not been employed so far.^[1] Nanohoops are a class of macrocycles with radially oriented π -systems, whose properties can be tuned by structural modification. By introducing RAGs, reversible electrochemical behavior can be obtained. Dihydrophenazine has already been used as a versatile RAG in organic battery electrode active materials, enabling high redox potentials.^[2] In this poster we will present the synthesis of diphenyldihydrophenazine-based nanohoops, their structural and optical properties, their electrochemical behavior, and their application and performance in organic half cells vs. lithium.

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ABSTRACTS OF POSTER PRESENTATIONS

P 22: Polymeric and covalent organic framework-based pyrene-4,5,9,10-tetraone positive electrodes for rechargeable aluminum batteries

Nico Kokott, Birgit Esser*

Institute of Organic Chemistry II and Advanced Materials

nico.kokott@uni-ulm.de

Rechargeable aluminum batteries (RABs) combine abundant, low-cost aluminum with a high theoretical volumetric capacity of the Al metal negative electrode (8040 mAh cm³). However, their development is limited by the scarcity of suitable positive electrode materials; state-of-the-art graphite typically provides only ~120 mAh g⁻¹.^[1] Redox-active carbonyl compounds offer high structural tunability and fast reaction kinetics, but small quinones such as pyrene-4,5,9,10-tetraone (PTO) suffer from dissolution in chloroaluminate electrolytes. Here, we compare two strategies for immobilizing PTO redox units: linear polymerization to poly(pyrene-4,5,9,10-tetraone) (PPTO)^[2] and incorporation into a crystalline PTO-based covalent organic framework (PTO-COF).^[3] Both materials are evaluated as positive electrodes in AlCl₃/EMIMCl aluminum half-cells. Solid-state ²⁷Al NMR, XPS, and EDX, supported by DFT calculations, reveal the reversible storage of AlCl₂⁺ charge carriers in PPTO and elucidate the charge-storage mechanism of polymeric carbonyl electrodes in RABs. PPTO and PTO-COF both show excellent cycling stability, confirming that polymer and framework immobilization effectively suppress dissolution. Incorporating carbon nanotubes into the PTO-COF electrode substantially improves electronic conductivity and rate capability. Comparison of the same redox motif in a linear polymer and a porous framework shows how molecular immobilization and electrode architecture govern dissolution, charge transport, kinetics, and electrochemical performance. These findings provide design principles for next-generation organic positive electrodes in rechargeable aluminum batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 23: Redox-active polymer cathode for sodium-inventory-controlled metal batteries

Nikhil Medhavi, Hakan Bildirir, Nagaraj Patil, Sergio Pinilla, Marta Liras, Rebeca Marcilla

Electrochemical Processes Unit, IMDEA Energy, Avda. Ramón de la Sagra 3, 28935 Móstoles, Spain

Photoactivated Processes Unit, IMDEA Energy, Avda. Ramón de la Sagra 3, 28935 Móstoles, Spain

rebeca.marcilla@energia.imdea.org

Organic||Ni(OH)₂ alkaline rechargeable batteries offer a safer and more sustainable route for aqueous energy storage, but their practical development requires organic anodes that combine fast kinetics, high active-material content, high mass loading, and reliable wide-temperature operation under mild alkaline conditions. Here, we introduce Aq-CMP@SR, a nanocarbon-assisted anthraquinone-conjugated microporous polymer (CMP) anode prepared by integrating a restrained SWCNT/rGO network in situ within a Suzuki–Miyaura-derived Aq-CMP framework. This hybrid design preserves the intrinsic anthraquinone redox chemistry while enhancing electrode-level electronic percolation, lowering ohmic and charge transfer resistances, accelerating apparent K⁺ diffusion, and increasing capacitive charge-storage contributions compared with non-hybrid Aq-CMP. Coupled with Ni(OH)₂ in 1 M KOH, Aq-CMP@SR delivers 143 mAh g⁻¹ at 80 wt% polymer content, with suppressed self-discharge and stable float-charge behavior. At high mass loading, the electrodes reach 10.1 mAh cm⁻² at 60 mg cm⁻² and still retain 4.6 mAh cm⁻² at 343 mA cm⁻². The cell also delivers ca. 37 Ah cm⁻² cumulative areal discharge capacity and operates from -45 to +75°C, achieving 111 mAh g⁻¹ at -45°C/1C and 122.4 mAh g⁻¹ at +75°C/300C. These results show that restrained nanocarbon hybridization enables mass-efficient, high-rate, and wide-temperature alkaline organic batteries under mild electrolyte conditions.

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ABSTRACTS OF POSTER PRESENTATIONS

P 24: Bipolar organic active materials for high-voltage redox flow batteries

Reinder Bouma, Edwin Otten

University of Groningen

r.h.bouma@rug.nl

The transition to renewable energy sources such as wind and solar requires large-scale, low-cost energy storage solutions. Redox flow batteries (RFBs) have emerged as a promising technology, offering high efficiency, simple design, and the ability to accommodate intermittent power supply. While commercial RFBs rely on metal ions such as vanadium, organic redox-active molecules could offer a more sustainable and cost effective alternative. These organic materials allow fine-tuning of key properties such as redox potential, chemical stability, and solubility.^[1] Moreover, organic solvents can achieve higher cell voltages due to their large electrochemical stability window (4-5 V) compared to aqueous systems (~1.5 V). This makes them attractive for developing higher energy density batteries. Despite advances in organic redox flow batteries (ORFBs), many challenges remain, including degradation and cross-contamination of redox-active materials.^[2] An approach to address cross-contamination is the development of symmetric ORFBs, where a single molecule is used on both sides of the battery.^[3] In order to facilitate both half-reactions, such symmetrical batteries require bipolar organics that are stable in three oxidation states. Rather than relying on trial-and-error approaches for the development of new bipolar RFB active materials, our research emphasizes the importance of understanding the chemical reactions that contribute to capacity fade. By strategically introducing both electron withdrawing and electron donating groups onto a benzene core, we systematically tune the electronic properties to achieve improved electrochemical stability and high cell potentials. By analyzing the degradation products formed during battery operation, we demonstrate how insights into electrolyte degradation can lead to development of new material, advancing the field towards more efficient and stable ORFBs.

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ABSTRACTS OF POSTER PRESENTATIONS

P 25: Polythiophene/non-fullerene donor-acceptor covalent conjugates for light energy harvesting technologies

Dr. Sana Iqbal

Lahore University of Management Sciences, LUMS, Lahore, Pakistan

s.iqbal@lums.edu.pk

The development of sustainable and durable energy-storage technologies requires organic electrode materials that combine high electrochemical activity with mechanical flexibility and structural stability. Here, we propose double-cable polymers (DCPs), originally developed as all-organic donor–acceptor (D–A) materials for light-energy harvesting, as a versatile platform for next-generation organic battery electrodes. Our DCPs consist of a polythiophene (PTh) backbone covalently integrated with redox-active non-fullerene acceptor (NFA) pendants. The covalent D–A architecture provides molecularly defined electronic communication between the polymer backbone and pendant functional units while avoiding the phase separation and uncontrolled organization commonly associated with physically blended organic materials. These materials have demonstrated efficient light harvesting and charge-generation properties, highlighting their ability to support charge transport through an extended conjugated framework. We propose translating this molecular design strategy from light-energy conversion to electrochemical energy storage by exploiting the redox activity of the pendant acceptor units as reversible charge-storage sites. In particular, PTh–PDI DCPs offer a promising architecture in which the conductive polymer backbone and redox-active PDI pendants are integrated within a single molecular framework. Further incorporation of carbon nanotubes and dynamic supramolecular interactions, such as quadruple hydrogen-bonding motifs, could generate interconnected electronic and chemical networks within a flexible ionogel-based electrode. This work establishes DCPs as a promising molecular platform beyond photocatalysis and photovoltaics and opens a new direction toward multifunctional, flexible, and potentially self-healing organic battery electrodes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 26: Ferrocene polymers for aqueous (zinc) battery cathodes

Sebastian Witt^{a,b}, Christian Stolze^{a,b,c,d}, Martin D. Hager^{a,b,c,d}, Ulrich S. Schubert^{a,b,c,d}

^aLaboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, 07743 Jena, Germany

^bCenter for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

^cHelmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstrasse 12-14, 07743 Jena, Germany

^dHelmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

sebastian.witt@uni-jena.de

Organic thin-film batteries are predominantly developed using non-aqueous electrolytes, whereas aqueous systems typically favor redox flow architectures. Ferrocene derivatives are well-established in aqueous redox flow batteries,^[1] yet their application in aqueous thin-film batteries remains scarce.^[2] This study explores the transferability of ferrocene chemistry from flow to thin-film configurations within aqueous zinc battery systems, targeting higher energy density. We investigated ferrocene polymers featuring amide functionalities to enhance hydrophilicity and compatibility with aqueous electrolytes. By systematically varying the alkyl tether length, we examined structure-property relationships governing cathode performance. Electrochemical evaluation indicated a strong correlation between tether length and cycling stability. While small tether length exhibited premature failure due to polarization, optimized architecture demonstrated viable cyclability, mitigating degradation mechanisms common in aqueous environments.^[3] This work presents a study on adapting known redox-active polymers for underrepresented battery formats. By demonstrating functional aqueous ferrocene thin-film electrodes, we highlight a novel application space distinct from conventional flow or lithium-organic systems. These findings suggest that molecular engineering can bridge the gap between flow and battery technologies, paving the way for sustainable energy storage solutions combining aqueous safety with organic thin-film versatility.

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ABSTRACTS OF POSTER PRESENTATIONS

P 27: Beyond TEMPO: Exploring alternative nitroxide scaffolds for aqueous organic redox flow batteries

Sebastien Gauden^a, Karim Boutamine^{a,b}, Patricia Bassil^b, Antoine Larman^b, Gilles Casano^a, Frédéric Favier^b, Steven Le Vot^b, Olivier Ouari^{a*}

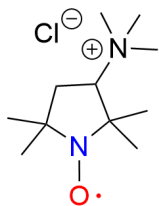
^aICR, Aix Marseille University, CNRS, Marseille, France

^bICGM, Université de Montpellier, CNRS, Montpellier, France

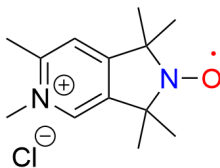
olivier.ouari@univ-amu.fr

Redox flow batteries (RFB) are a promising solution for the stationary storage of electricity generated from intermittent sources such as solar and wind. Currently, the most widely deployed technology relies on aqueous vanadium-based electrolytes.. However, the high cost of vanadium, limited energy density and the use of corrosive solutions push on the search of alternatives for the large scale implementation of these systems. In this context, organic redox-active electrolytes have emerged as attractive alternatives for developping safer, more sustainable, and potentially more cost-effective RFB. Among the various organic redox couples investigated, the N-oxoammonium/nitroxide couple is particularly promising as a positive electrolyte (posolyte) for aqueous organic redox flow batteries (ORFBs), owing to its fast and reversible redox chemistry. Nevertheless, the long-term stability of these systems remains a major limitation. While TEMPO-based nitroxides are generally stable persistent radicals in aqueous solution at neutral pH, the stability of the corresponding N-oxoammonium species is less clear. Understanding these processes is therefore essential for improving the lifetime and performance of nitroxide-based ORFBs.^[1] To date, most efforts to address this issue have focused on the structural modification of TEMPO derivatives to enhance the stability of the corresponding N-oxoammonium species. In contrast, the broader structural diversity of nitroxide radicals remains poorly explored. In this work, we investigate two alternative nitroxide scaffolds as potential posolytes for aqueous ORFBs, with the aim of assessing their redox properties and long-term chemical stability and identifying structural features that may contribute to improved battery performance..^{[2][3]} (Fig 1)

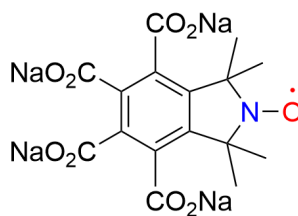
ABSTRACTS OF POSTER PRESENTATIONS



TMA-Proxyl



PPO



TC-TMIO

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Figure 1: structure of new posolytes for AORFB

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ABSTRACTS OF POSTER PRESENTATIONS

P 28: Porphyrinoids as universal cathodes for monovalent, divalent, and trivalent metal-ion batteries

Svetlana Klyatskaya^a, Masoumeh Zakerighadi^a, Mario Ruben^{a,b,c}

^aInstitute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

^bInstitute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

^cCentre Européen de Sciences Quantiques (CESQ), Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Strasbourg, France

svetlana.klyatskaya@kit.edu

Porphyrinoids, macrocyclic organic compounds derived from porphyrins, have emerged as promising materials in battery applications due to their unique redox properties, structural tunability, and metal-coordination capabilities. Their use in rechargeable batteries offers a sustainable alternative to conventional inorganic materials. These materials could help develop high-capacity, stable, and environmentally friendly batteries for energy storage. Key Advantages: High Redox Activity – Enables efficient charge storage and discharge cycles; Tunable Electronic Properties – Structural modifications allow for enhanced conductivity and stability; Metal Coordination Capability – Supports incorporation of transition metals, improving electrochemical performance; Sustainability – Organic and bio-derived porphyrinoids provide an eco-friendly alternative. The study explores their potential as universal cathodes, meaning they can work with different metal ions: Monovalent (e.g., Li, Na, K); Divalent (e.g., Mg²⁺, Zn²⁺, Ca²⁺) ; Trivalent (e.g., Al³⁺).

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ABSTRACTS OF POSTER PRESENTATIONS

P 29: Pyrazine–quinone organic cathodes for high-energy lithium, zinc, and proton batteries

Svit Menart^{1*}, Klemen Pirnat¹, Robert Dominko^{1,2,3}

¹Department of Materials Chemistry, National Institute of Chemistry, 1000 Ljubljana, Slovenia

²Faculty of Chemistry and Chemical Technology, University of Ljubljana, 1000 Ljubljana, Slovenia

³Alistore-European Research Institute, 80039 Amiens, France

svit.menart@ki.si

Organic electrode materials offer a sustainable alternative to resource-scarce inorganic cathodes; however, achieving high energy density, good long-term stability, and simple synthesis procedures remains a significant challenge. Combining pyrazine and quinone structural motifs represents a promising strategy toward high-energy organic materials. Here, we present a facile synthesis strategy utilizing a sodium rhodizonate precursor to simultaneously incorporate pyrazine and quinone motifs into scalable organic architectures. In lithium batteries, these materials yield high energy densities up to 860 Wh kg⁻¹ with 82% capacity retention after 400 cycles at 50 mA g⁻¹ [1]. To push performance further, we report the first combination of bipyrazino and catechol redox-active motifs within a single organic framework. In lithium half-cells, this structural design delivers a specific capacity of 281 mAh g⁻¹ at 2.50 V vs. Li/Li⁺, with voltage-window optimization yielding 96% capacity retention over 190 cycles [2].

In aqueous zinc-ion batteries (ZIBs), the materials maintain high energy densities up to 280 Wh kg⁻¹, while novel hexaazatriphenylene (HAT)-derived variants achieve practical reversible capacities up to 503 mAh g⁻¹. The bipyrazino–catechol design delivers 298 mAh g⁻¹ in ZIBs with an exceptionally high average discharge voltage for n-type material of 1.00 V vs. Zn/Zn²⁺. Mechanistic insights from ex situ FT-IR, pH-dependent cycling, and DFT calculations reveal that its redox chemistry in aqueous ZIBs is predominantly driven by proton (H⁺) coordination rather than Zn²⁺ insertion, further validated by a high capacity of 287 mAh g⁻¹ in a pure proton battery setup (H₂SO₄, pH = 1).

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ABSTRACTS OF POSTER PRESENTATIONS

P 30: Development of dihydroxysulfonatobenzoate salts as organic electrode materials for li-ion batteries

Yannis Zekhenine^{1,2}, Etienne Lepoivre¹, Lionel Dubois², Thibaut Gutel¹

¹Univ. Grenoble Alpes, CEA, LITEN, DEHT, 38000 Grenoble, France

²Univ. Grenoble Alpes, CEA, IRIG, DIESE, 38000 Grenoble, France

thibaut.gutel@cea.fr

N-type organic electrode materials should offer a cost-effective and environmental friendly alternatives for Li-ion battery. Indeed these products can be prepared using green chemistry from low cost (bio-based) precursors. But until now, their implementation in full prototypes is still challenging especially due to their high solubility in liquid electrolytes but also because of their low electronic conductivity and their instability in reduced state in (even dry) air. Only few examples of lithiated air-stable compounds such as tetralithium 2,5-dihydroxy-1,4-benzenedisulfonate (Li₄-p-DHBDS),^[1] magnesium (2,5-dilithium-oxy)-terephthalate (MgLi₂-p-DHT),^[2] or tetra lithium salt of the naphthazarin dimer (DNP-Li)^[3] have been reported up to now as positive electrode materials. In order to demonstrate the interest of organic battery technology, our group assembled first Li-ion prototypes (multi-layer prismatic cell of 160mAh) using MgLi₂-p-DHT versus graphite based electrodes which show some promising electrochemical performances with high capacity retention at high C-rate (>70% at 2C) or after 250 cycles (>80% of initial capacity) and a proven energy density of 60Wh.kg⁻¹ at cell level. To go one step further, a new generation of organic active materials based on dihydroxysulfonatobenzoate salts have been developed. Their syntheses and physico-chemical characterizations will be presented. Indeed their electrochemical properties appear very interesting for applications as positive electrode materials with some average redox potentials above 3V vs Li⁺/Li and some stability against air in reduced lithiated states.

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ABSTRACTS OF POSTER PRESENTATIONS

P 31: Pyrrolo[3,2-b]pyrrole polymers and COFs as cathode materials for organic batteries

Tobias Wasserrab¹, Wolfgang Kies², Oliver Dumele², Birgit Esser^{1*}

¹Institute of Organic Chemistry II and Advanced Materials, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany; CELEST Green Energy Lab Ulm, Ulm University, Lise-Meitner-Str. 16, 89081 Ulm, Germany

²Institute of Organic Chemistry, University of Cologne, Greinstrasse 4, 50939 Cologne, Germany

tobias.wasserrab@uni-ulm.de

Metal oxide-based intercalation materials are nowadays widely used as cathodes in lithium-ion batteries and show great performance in cycling stability and high capacity.^[1] In the last years organic redox-active molecules have emerged as an alternative to the typically employed inorganic materials. Organic molecules that can undergo reversible oxidation are promising candidates for cathode materials.^[2] However, the performance of organic materials is limited by their cycling stability and rate performance at high voltages of more than 3.4 V versus Li/Li+.^[3] In this study, a conjugated polymer and covalent organic frameworks (COF), with dihydropyrrolo[3,2-b]pyrrole (DHPP) as the redox active unit, are investigated as a possible cathode material for organic battery cells. The tetraphenyl-substituted DHPP **1** can undergo two reversible oxidations, which makes it a promising candidate for this application (Figure 1). To address the issue of dissolution or degradation in the organic electrolyte, as well as enhance the cycling stability, the DHPP motif is incorporated into a polymer backbone or as linker in a COF. Herin, we compare the properties of DHPP polymers and COFs in lithium half-cells and investigate how structural variations, such as porosity, translate into differences in electrochemical performance.

ABSTRACTS OF POSTER PRESENTATIONS

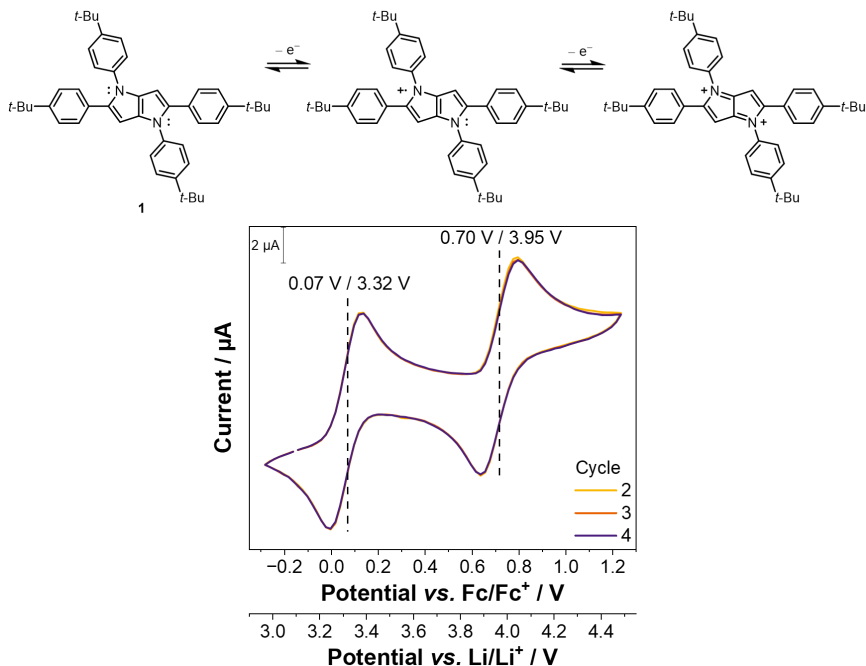


Figure 1: Cyclic voltammogram of tetraphenyl-substituted DHPP **1** in CH_2Cl_2 .

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ABSTRACTS OF POSTER PRESENTATIONS

P 32: Dual-redox phenazine-derived cathodes for Zn and Li batteries

Vladyslav Yatsenko^{a,b}, Klemen Pirnat^a, Svit Menart^a, Robert Dominko^{a,b,c}

^aNational Institute of Chemistry, Hajdrihova 19 SI, Ljubljana 1000, Slovenia

^bFaculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113 SI, Ljubljana 1000, Slovenia

^cAlistore-European Research Institute, CNRS FR 3104, Hub de l'Energie, Rue Baudelocque, 80039 Amiens, France

Vladyslav.Yatsenko@ki.si

Keywords: Phenazine-2,3,7,8-tetramine-based materials, organic cathodes, pyrazine, quinone, Zn battery, Li battery.

Small organic molecules are attracting increasing interest as sustainable electrode materials for next-generation rechargeable batteries due to their structural versatility, low cost, and abundant raw material sources. Nevertheless, their practical implementation is often hindered by limited electrical conductivity and dissolution in the electrolyte, resulting in low active-material utilization and poor cycling stability. Herein, we report a simple synthetic approach to organic cathode materials that integrate pyrazine and quinone redox-active motifs using readily accessible starting compounds. The resulting phenazine-based materials were obtained through a condensation reaction and investigated as cathodes in zinc- and lithium-based battery systems. The rigid fused aromatic frameworks exhibit low solubility in electrolytes due to strong π - π stacking interactions, contributing to improved cycling stability. In aqueous Zn batteries, 9,11,13,22,24,26-hexaza-tetrabenzo[a,c,p,r]heptacene (HATBH) delivered 148 mAh g⁻¹ at 100 mA g⁻¹ with excellent cycling stability, while nitrogen-enriched 9,26-dihydro-9,11,13,22,24,26-hexaza-tetrapyrido[3,2-a:2',3'-c:3',2'-p:2',3'-r]heptacene (DHATPH) reached 215 mAh g⁻¹. Electrochemical and spectroscopic analyses indicate predominantly proton-coupled electron-transfer charge-storage mechanisms. Furthermore, oxidation of HATBH with potassium dichromate introduced additional quinone redox centers, increasing the capacity to 302 mAh g⁻¹ at 100 mA g⁻¹, though with reduced cycling stability. These results demonstrate that molecular engineering of pyrazine- and quinone-containing phenazine derivatives provides a viable strategy for tuning the capacity and durability of sustainable organic cathodes. ^[1]

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ABSTRACTS OF POSTER PRESENTATIONS

P 33: Pyridinium-Substituted molecules as anodes for sustainable all-organic batteries

Xhesilda Fataj^{a,b,d}, Andreas J. Achazi^d, Christian Stolze^{a,b,d}, Doreen Mollenhauer^{b,d}, Martin D. Hager^{a,b,c,d}, Ulrich S. Schubert^{a,b,c,d}

^aLaboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

^bCenter for Energy and Environmental Chemistry Jena (CEEC Jena), Philosophenweg 7a, 07743 Jena, Germany

^cHelmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), 14109 Berlin, Germany

^dHelmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstr. 12-14, 07743 Jena, Germany

xhesilda.fataj@uni-jena.de; ulrich.schubert@uni-jena.de

The development of sustainable energy-storage systems is essential for reducing the environmental impact of modern technologies. Organic batteries based on redox-active molecules offer a promising alternative to conventional lithium-ion batteries by reducing reliance on critical metal resources. ^[1]

This work investigates pyridinium-substituted benzothiazole, benzoxazole, and benzimidazole derivatives as building blocks for polymeric electrode materials. Combined theoretical and experimental screening identified pyridinium-benzoxazole as the most promising candidate due to its favorable electrochemical properties and redox stability. ^[2,3] It was incorporated into a polymer backbone via radical polymerization, yielding poly(4-(benzoxazol-2-yl)-1-(4-vinylbenzyl)pyridinium chloride) (PBO-Cl⁺), with a theoretical specific capacity of 76.8 mAh g⁻¹ for the first redox process. PBO-Cl⁺ was evaluated as an anode in all-organic batteries using TEMPO-based cathode materials. ^[4] It showed stable performance in both organic and aqueous electrolytes, reaching 99% capacity utilization at 1C in the first cycle in 1 M LiClO₄/CH₃CN and retaining more than 50% of its capacity after 100 cycles. ^[4] Furthermore, the polymer counterion and electrolyte composition strongly influenced its redox behavior, coulombic efficiency, and capacity utilization. ^[5]

Overall, this work provides valuable insights into the design of new organic anode materials and contributes to expanding the range of sustainable electrode materials available for next-generation all-organic metal-free battery technologies.

ABSTRACTS OF POSTER PRESENTATIONS

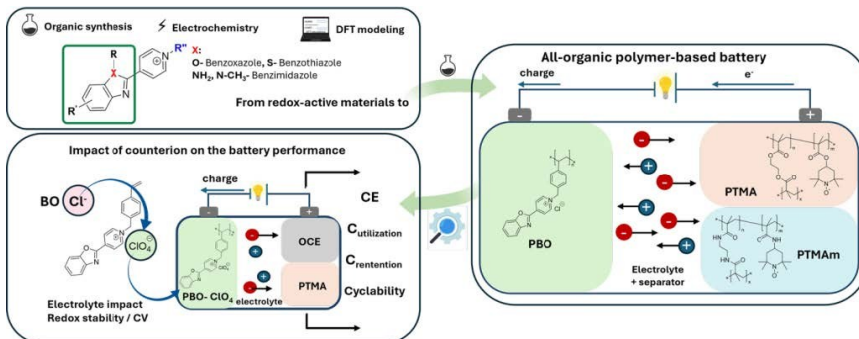


Figure 1. Schematic representation of the research presented in this abstract. Three groups of redox-active molecules were screened using combined experimental and theoretical approaches (left). The best-performing benzoxazole-based molecule was selected as an anode material for all-organic batteries with TEMPO-based cathodes in organic and aqueous electrolytes (right). Finally, the effects of the counterion and electrolyte composition on electrochemical performance were investigated.

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ABSTRACTS OF POSTER PRESENTATIONS

P 34: Phenothiazine-based hypercrosslinked polymers as high-voltage organic cathodes for lithium batteries

Yogajivan Rout

IMDEA Energy Institute

yogajivan.rout@energia.imdea.org

The increasing global energy demand, geopolitical uncertainties, and concerns over fossil-fuel dependence have intensified the need for sustainable and resource-secure energy-storage technologies. In this context, organic batteries are attracting increasing attention because redox-active organic materials can be constructed from abundant elements and offer extensive structural and electrochemical tunability. Among them, p-type organic cathodes are particularly attractive because of their relatively high operating potentials and rapid redox kinetics. ^[1] IEP-29 is a phenothiazine-based hypercrosslinked polymer synthesized via Friedel-Crafts knitting polymerization. ^[2] As a lithium-battery cathode, IEP-29 delivered a specific capacity of 106 mAh g⁻¹ at 0.5 C with an average discharge potential of 3.6 V vs Li/Li⁺. It retained 60 mAh g⁻¹ at 15 C and 79% of its capacity after 1000 cycles at 2 C. Despite this promising performance, IEP-29 exhibits a relatively low Brunauer-Emmett-Teller surface area of approximately 8 m² g⁻¹, suggesting that further gains may be possible by improving pore accessibility and redox-site utilization. Building on this observation, our ongoing work investigates how the synthetic environment can be used to control the porous structure of phenothiazine-based hypercrosslinked polymers. A range of catalytic systems, reaction conditions, media, and synthetic approaches are currently under evaluation, with the aim of identifying the key parameters governing network formation, accessible porosity, and electrochemical response. Initial screening indicates that the textural and electrochemical properties are highly sensitive to these synthetic variables. This work seeks to establish broader synthesis-structure-property relationships that can guide the development of high-voltage, durable organic cathodes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 35: Porous covalent organic frameworks as active battery electrode materials

Oliver Dumele

Institute of Organic Chemistry, University of Cologne, Greinstrasse 4, 50939 Cologne, Germany

odumele@uni-koeln.de

Constructing Organic Covalent Frameworks (COFs) from advanced molecular building blocks can achieve novel functional materials.^[1,2] Inspired by the porous and insoluble structure of COFs, we developed a series of all-organic electrode materials to be used as cathode materials for various Li and Mg-based cells in collaboration with the group of Birgit Esser (Ulm Univ). We found that p-type COF can reach average discharge potentials of 3.9 V (vs. Li/Li⁺) and that porous materials show better performance in battery cells as non-porous amorphous polymers consisting of the same redox-active monomeric unit.

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ABSTRACTS OF POSTER PRESENTATIONS

P 36: A naphthalene diimide based neutral pH hybrid redox flow battery

A. Kumar^{1,2}, M. D. Hager^{1,2,3,4}, U. S. Schubert^{1,2,3,4*}

¹Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

²Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

³Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

⁴Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

ulrich.schubert@uni-jena.de

Redox flow batteries (RFBs) are promising candidates for large scale energy storage owing to easy scalability and decoupled energy and power density. The aqueous vanadium RFBs represent state-of-the-art among all RFB technologies; however, it utilizes highly corrosive and toxic electrolytes ^[1]. Currently, aqueous organic RFBs are emerging as sustainable alternatives owing to use of highly abundant redox active organic materials (ROMs) which offer tunable properties based on molecular architecture. ROMs offer practical application under neutral pH aqueous conditions in RFBs and feature a broad library of molecular structures such as 2,2,6,6-tetramethylpiperidinyloxy, ferrocene, viologen, and naphthalene diimide ^[2]. The water solubility, redox potential, and chemical stability of ROMs are tuned by tailoring of molecular cores with ionic functional groups. Moreover, ROMs are limited by varying solubilities in charged and uncharged state, where the lower water solubility state governs the achievable energy density of the solution RFBs ^[3]. In this contribution, we present for the first time a neutral pH aqueous hybrid RFB to state this issue with reversible assembly and disassembly of asymmetric naphthalene diimide (ANDI) ROMs. The ANDI ROMs were synthesized by first asymmetrically functionalizing naphthalene dianhydride core with hydrophobic alkyl chain and in the second step with hydrophilic side chains bearing quaternary ammonium or zwitterionic functionalities. The side chain length and hydrophilicity offer tuning of π - π stacking and water solubility. The ANDI molecules revealed robust electrochemical properties with reversible two-electron kinetics and the hybrid RFB demonstrated superior performance with average coulombic efficiency of >97% and capacity retention per cycle of >99.75% over 80 charge and discharge cycles.

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ABSTRACTS OF POSTER PRESENTATIONS

P 37: Harnessing porous solids for high energy density redox flow batteries

Ferit Begar, Edwin Otten

Nijenborgh 3, 9747 AG Groningen, The Netherlands

Redox flow batteries (RFBs) store electrical energy in redox-active species dissolved in electrolyte solutions that are circulated through an electrochemical cell and stored in external tanks. However, the limited solubility of redox-active materials imposes a fundamental constraint on the achievable energy density of conventional RFBs, hindering their application in large-scale energy storage. Redox-targeting flow batteries (RTFBs) offer a promising strategy to overcome this limitation by employing a soluble redox mediator to shuttle electrons between the electrochemical cell and a redox-active solid stored in the tank. Because solid-state materials can provide substantially higher redox-active site densities than dissolved species, RTFBs can potentially achieve higher energy densities without relying on highly soluble active materials.

In this project, we investigate porous redox-active solids, including Metal–Organic Frameworks (MOFs), Covalent Organic Frameworks (COFs), and Porous Organic Polymers (POPs), as redox targets for RTFBs. Redox-active monomers are incorporated into these porous materials through covalent or coordination bonds, enabling systematic investigation of how pore structure and accessibility influence electron transfer between the soluble mediator and the solid-state redox sites. In particular, we aim to elucidate the relationship between porosity, redox-site accessibility, and the depth and rate of redox targeting.

The electrochemical performance of RTFBs incorporating these porous redox-active materials will be evaluated in terms of capacity utilization, energy density, rate capability, and long-term cycling stability. This work aims to establish design principles for porous redox targets and advance the development of high-energy-density flow batteries for large-scale energy storage.

ABSTRACTS OF POSTER PRESENTATIONS

P 38: 4-Benzoylpyridinium based redox-active polymers for redox-targeting flow battery applications

Linus Altemöller, Mariano Grünebaum, Bart Jan Ravoo

Organisch-Chemisches Institut, University of Münster

linusaltemoeller@uni-muenster.de

Redox-targeting flow batteries (RTFBs) overcome the solubility limit of flow batteries by storing additional energy into an insoluble material, the solid-booster, in the tank. Despite this advantage, the library of successfully implemented redox-active polymers (RAPs) as solid-boosters remains highly limited. This work presents a solid-booster based on the low-potential N-alkyl-4-benzoylpyridinium (4-BP) moiety ($E_{1/2, \text{red}} = -1.08 \text{ V vs Fc/Fc}^*$) as an alternative to viologen ($E_{1/2, \text{red}} = -0.83 \text{ V vs Fc/Fc}^*$). Two distinct N-methyl and N-isopropyl 4-BP polymer particle architectures were synthesized. Their electrochemical performance was evaluated in an Hcell setup, utilizing single and dual-shuttle systems under various conditions. The N-isopropyl based systems demonstrated a high polymer utilization of initial >90% and maintaining >85% after 80 cycles. Furthermore, the battery exhibits stable performance over 220 cycles without noticeable capacity fading. This work expands the limited palette of polymer based solid-boosters, offering robust and low-potential 4-BP based RAPs for RTFBs.

ABSTRACTS OF POSTER PRESENTATIONS

P 39: Single-crystal copper current collector for stable anode-free lithium metal batteries

Seung Heon Choi¹, Min Jun Hwang², Ho Seok Park^{1,2*}

¹School of Future Energy Engineering, Sungkyunkwan University (SKKU), Suwon 440-746, Republic of Korea

²School of Chemical Engineering, Sungkyunkwan University (SKKU), Suwon 440-746, Republic of Korea; SAIHST, Sungkyunkwan University, Suwon, Republic of Korea

ash7998@skku.edu

Anode-free lithium metal batteries are considered a promising platform for achieving high energy density because they eliminate excess lithium metal and inactive anode materials from the initial cell configuration. However, their practical implementation remains severely limited by the low reversibility of lithium plating and stripping on conventional polycrystalline Cu current collectors. Variations in crystallographic orientation, grain boundaries, surface defects, and local surface energy create spatially heterogeneous nucleation environments, resulting in non-uniform current distribution, localized lithium accumulation, dendritic growth, and continuous formation of inactive lithium and unstable solid–electrolyte interphases. Here, we propose a single-crystal copper current collector as a structurally defined platform for regulating lithium nucleation and growth in anode-free cells. Unlike conventional polycrystalline Cu, the single-crystal Cu substrate provides a crystallographically uniform surface with substantially reduced grain-boundary-induced heterogeneity. This homogeneous interfacial environment is expected to minimize local variations in lithium nucleation barriers and surface transport behavior, thereby promoting more spatially uniform nucleation and controlled lateral growth of deposited lithium. The uniform crystal orientation can also reduce localized current-density hotspots and facilitate the formation of a dense and continuous lithium layer with reduced surface area. Through this crystallographic regulation of the current-collector interface, uneven lithium deposition, dendrite formation, and irreversible lithium loss can be mitigated during repeated plating and stripping. Consequently, the single-crystal Cu current collector provides a materials-level strategy for improving interfacial stability, lithium utilization, and cycling durability without introducing additional coating layers or complex three-dimensional structures. This work highlights the importance of current-collector crystallinity in governing lithium electrodeposition and provides a fundamental design direction for developing durable, high-energy-density anode-free lithium metal batteries.

ABSTRACTS OF POSTER PRESENTATIONS

P 40: Solid-state NMR for batteries and battery materials: From structural characterization to mechanistic understanding

Buyun Gao, Eike Brunner

Technische Universität Dresden

The development of next-generation and organic battery technologies requires a molecular-level understanding of the materials and the electrochemical processes governing their operation. Solid-state nuclear magnetic resonance (ssNMR) spectroscopy has emerged as a powerful, non-destructive tool to provide information on local chemical environments, coordination geometries, site defects, and structural evolution during or after reactions.

In this work, we demonstrate the versatility of ex situ ssNMR through three representative case studies. First, we utilized ^{13}C MAS NMR to precisely characterize the local connectivity of newly synthesized covalent organic frameworks (COFs), confirming the formation of the desired linkages. Second, we employed ^{77}Se ssNMR to demonstrate how local structural information can be used to distinguish the reaction pathway in battery. Finally, ^{27}Al ssNMR will illustrate how to identify the actual charge carrier in aluminium batteries, providing direct experimental insight into the underlying storage mechanism.

Building upon these ex situ case studies, the principles and experimental designs of in situ and operando NMR techniques for electrochemical systems will be also introduced. Particular attention will be given to the development of (ss) NMR-compatible electromechanical cell design, which demonstrates how electrochemical reactions can be monitored under operating conditions while maintaining accurate electrochemical control. Such advances enable real-time observation of electrolyte evolution, reaction intermediates, and electrochemical kinetics in real time.

In summary, this presentation demonstrates how advanced ssNMR configurations bridge the gap between static structure characterization and dynamic mechanistic understanding. Moving from ex situ characterizations to real-time observations provides a powerful tool, offering a pathway to establish structure-property relationships. These insights offer guidance for the rational design of next-generation sustainable energy storage and high-performance organic batteries and their materials.

ABSTRACTS OF POSTER PRESENTATIONS

P 41: Developing an online ^{19}F NMR workflow for monitoring degradation in organic redox flow batteries

Bhawna Choudhary, Edwin Otten

Stratingh Institute for Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

b.choudhary@rug.nl

Organic redox flow batteries (RFBs) are promising for large-scale energy storage because their properties can be tuned through molecular design. However, their practical use is still limited by capacity fade arising from incompletely understood chemical degradation processes. Standard electrochemical measurements provide overall performance data, but they do not give direct information about changes at the molecular level.

Here, we develop an online operando ^{19}F NMR workflow to monitor electrolyte composition during electrochemical cycling. By introducing fluorine-containing tags into redox-active molecules, ^{19}F NMR enables selective detection of these species in real time. Fluorinated supporting electrolyte components can provide additional insight into chemical changes ^[1]. A benchtop NMR spectrometer is integrated with electrochemical cells, enabling continuous electrolyte flow through the NMR detection region during cycling ^[2].

Initial experiments evaluated the suitability of the setup for long-term operando measurements, including external lock stability, chemical shift behavior, spectral resolution and sensitivity. These studies demonstrated stable and reproducible ^{19}F NMR measurements. The workflow is subsequently applied to fluorinated phenothiazine derivatives during electrochemical cycling. Initial measurements reveal changes in the ^{19}F NMR response, including decreases in or disappearance of resonances depending on the electrochemical state and the occasional appearance of additional signals. Ongoing analysis aims to establish the molecular origin of these changes and their relationship to electrochemical processes and degradation pathways.

Overall, this work establishes an operando platform for correlating electrochemical behavior with molecular-level changes in organic redox-active materials, supporting the development of more stable electrolytes and longer-lasting organic RFB systems.

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ABSTRACTS OF POSTER PRESENTATIONS

P 42: Flow battery electrolyte parameter prediction based on state-of-charge measurements

Christian Stolze^{1,2,3}, Ivan A. Volodin^{1,2}, Philip Rohland^{1,2}, Jan P. Meurer^{1,2}, Karina Zub¹, Oliver Nolte^{1,2}, Martin D. Hager^{1,2,3}, Ulrich S. Schubert^{1,2,3}

¹Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

²Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

³Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

⁴Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

christian.stolze@uni-jena.de

The state-of-charge (SOC), and the state-of-health (SOH) of the electrolytes in a redox flow battery (RFB) are among the most important physicochemical parameters of this battery type. A multitude of methods have been proposed to enable their cost-efficient, accurate, and reliable measurement. Nearly all these methods make use of the strong impact of SOC/SOH changes on nearly all other physicochemical parameters of an electrolyte.^[1] Such methods follow a common scheme: (1) Investigate the quantitative relationship between electrolyte SOC/SOH and another parameter (e.g., capacity, conductivity, spectral properties, etc.), (2) establish a calibration curve or computational model (e.g., Kalman-filter, ML, etc.) that enables prediction of the SOC/SOH from this parameter, and (3) monitor the other parameter during battery operation to predict the SOC/SOH using the established calibration. While calibration-based methods can be accurate and reliable for specific electrolytes, they require frequent re-calibration and corrections to account for parameter interdependencies (e.g., temperature variations).

With the introduction of amperometric techniques, a class of absolute SOC/SOH measurement methods based on simple electrochemical principles became available. They are accurate (absolute errors < 1%), temperature-independent, and calibration-free. Consequently, they strip away many of the complex interactions that need to be accounted for in other techniques.^[2, 3] In addition, they enable an inversion of the prediction route: With a calibration-free and accurate SOC/SOH measurement, one may predict other parameters such as electrolyte capacity, electrolyte conductivity, and many other parameters.^[3]

This poster illustrates the working principle of amperometric techniques and outlines a path towards a comprehensive methodological toolbox for RFB electrolyte monitoring and investigation.

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ABSTRACTS OF POSTER PRESENTATIONS

P 43: An operando benchtop magnetic resonance toolbox for studying redox flow batteries

G. A. Silva Testa^a, M. Damhuis^b, Tom Speelman^c, Kim Baas^a, J. C. Martínez López^d, M. Santos Rodríguez^d, Á. E. Lozano^d, C. Álvarez^d, J. Carretero Gonzalez^d, H. A. A. W. Elemans^e, E. W. Zhao^a

^aMagnetic Resonance Research Center, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

^bMolecular Nanofabrication (MNF), University of Twente, Hallenweg 23, 7522 NH Enschede, The Netherlands

^cTheoretical and Computational Chemistry, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

^dInstitute of Polymer Science and Technology, ICTP, CSIC, C/Juan de la Cierva 3, Madrid 28006, Spain

^eSpectroscopy and Catalysis, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

giu.silvatesta@ru.nl; evanwenbo.zhao@ru.nl

Redox flow batteries (RFBs) are promising for grid-scale energy storage, but molecular processes occurring during operation remain difficult to probe directly. While operando nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) spectroscopy can provide valuable mechanistic insight, access to high-field instrumentation remains limited. Here, we demonstrate how benchtop NMR and EPR can be used to study complementary processes in operating RFBs.

First, we applied ⁷Li NMR to investigate Li⁺ transport through a new class of ion-selective fluorine-free membranes. By monitoring changes in ⁷Li signal intensity and chemical shift during electrochemical cycling, Li⁺ transport and concentration changes could be followed directly, while also retrieving information on the battery's state of charge. We then coupled benchtop NMR and EPR to simultaneously monitor diamagnetic and paramagnetic species in a methyl viologen (MV²⁺)/TEMPOL RFB. In this study, ¹H NMR followed the evolution of MV²⁺ during chargedischarge, while EPR detected the corresponding formation and consumption of MV^{•+} radical cations. The electronic structure and apparent concentration of the radicals were quantified under operating conditions.

Together, these results show that benchtop magnetic resonance provides an accessible operando platform for following ion transport, redox-state changes, and radical intermediates in flow batteries, and can be extended to a broad range of electrochemical systems.

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ABSTRACTS OF POSTER PRESENTATIONS

P 44: Chloride compatibility of organic battery electrode materials

Isabel H. Morhenn, Birgit Esser

Institute of Organic Chemistry II and Advanced Materials, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

isabel.morhenn@uni-ulm.de

The lithium-ion battery (LIB) is today's state of the art for portable energy storage.^[1] In LIBs the Li^+ cation travels back and forth from the cathode to the anode in a so-called rocking-chair configuration. Chloride-ion batteries (CIBs) work in a similar way, expect that the Li^+ cation is replaced by a Cl^- anion as the shuttling ion.^[1] During charging and discharging, LIBs and other metal-ion batteries can undergo dendrite-formation, which leads to short circuits. This is not the case with CIBs, due to the absence of metals. Another advantage of CIBs over LIBs is the high abundance of chloride anions on earth. Therefore, CIBs have great potential as a low-cost replacement of LIBs.^[1] Being excellent candidates for insertion of anions upon oxidation, p-type organic electrode materials are great candidates for CIBs.^[2] Their properties can easily be modified by structural tuning.^[2] However, identifying suitable electrode materials for CIBs presents a challenge. In this work we employed spectroelectrochemical measurements to determine the chloride compatibility of a selection of organic battery electrode materials. Viologen-, phenothiazine- and dihydrophenazine-based molecules (Figure 1) were chosen due to their good characteristics as p-type electrode materials, such as a good cycling stability.^[2,3] All show two reversible one-electron redox reactions comprising the dication, radical cation and neutral state.^[2,3] We observed the changes in electronic structure with UV/Vis/NIR spectroscopy and cyclic voltammetry and how it is effected by the presence of chloride ions. This enables selecting the most promising candidates to further pursue in CIBs.

ABSTRACTS OF POSTER PRESENTATIONS

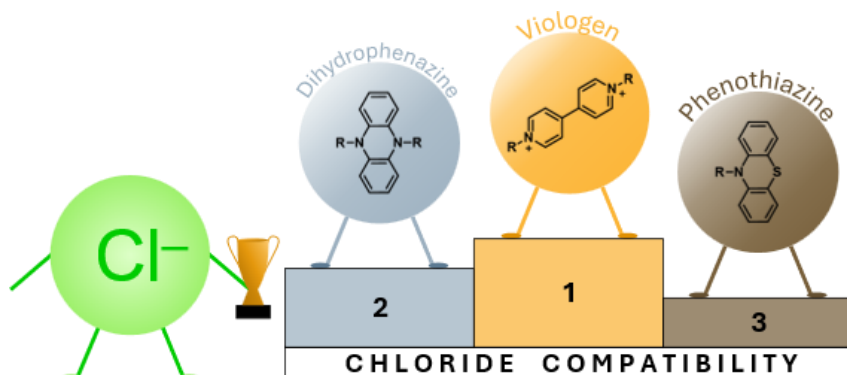


Figure 1: Investigating the chloride compatibility of the organic electrode materials viologen, dihydrophenazine and phenothiazine

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ABSTRACTS OF POSTER PRESENTATIONS

P 45: Beyond active material design: The critical role of conductive carbon networks in organic electrodes

Masoumeh Zakerighadi¹, Saibal Jana¹, Ebrahim Abouzari-Lotf^{2,3*}, Svetlana Klyatskaya¹, Wolfgang Wenzel¹, Mario Ruben^{1,4,5*}

¹Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

²Helmholtz Institute Ulm (HIU), Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm, Germany

³Trinseo Deutschland Anlagengesellschaft mbH

⁴Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

⁵Centre Européen de Science Quantique (CESQ), Institut de Science et d'Ingénierie Supramoléculaires (ISIS), 8 allée Gaspard Monge BP 70028, 67083 Strasbourg Cedex, France

mario.ruben@kit.edu; eabouzarilotf@trinseo.com

Organic electrode materials have attracted significant interest as sustainable alternatives for nextgeneration mono and multivalent ion batteries including Li, Na, K, Mg, and Zn ion systems, owing to structural diversity, synthetic tunability and potential for multi-electron redox reactions. Despite advantages, their practical implementation remains hindered by low electronic conductivity, dissolution in electrolytes and limited cycling stability. Considerable efforts have been devoted to overcoming these limitations through molecular engineering of redox-active materials, resulting in substantial improvements in electrochemical performance ^[1]. In contrast, role of conductive additives, despite being essential for charge transport, has received comparatively little attention and is treated as an inert formulation component. We demonstrate that conductive additive engineering is a critical and overlooked parameter governing electrochemical performance of electrodes. Using copper porphyrin (CuDEPP) as a model active material, we systematically investigate the influence of diverse conductive carbons on electrode performance in lithium and sodium-ion batteries ^[2]. Our results reveal that conductive network efficiency varies significantly among carbon additives, enabling comparable electrochemical performance to be achieved with substantially lower carbon loadings when appropriate conductive additives are employed. Among the conductive additives, graphene nanoplatelets enable efficient electronic pathways and deliver highest capacities at different current densities, reaching **204 mAh⁻¹** in Li and **229 mAh g⁻¹** in Na-ion cells. These findings are supported by theoretical calculations, electrochemical impedance and extended cycling, demonstrating an optimal balance of conductive additive content and morphology is essential for long-term stability and

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highrate performance.

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ABSTRACTS OF POSTER PRESENTATIONS

P 46: Study of polyphosphazene-based organic radical polymers via electron paramagnetic resonance spectroscopy

Natalia Gurinovich^{1,2}, Josef Granwehr^{1,2}, Lucas Marquart³, Gunther Brunklaus³, Rudiger-A. Eichel¹

¹Institute of Energy and Climate Research - Fundamental Electrochemistry (IET-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

²Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, 52056 Aachen, Germany

³Helmholtz-Institute Münster (IMD-4), Forschungszentrum Jülich GmbH, 48149 Münster, Germany

n.gurinovich@fz-juelich.de

Investigation of functioning of new electrode materials plays an important part in development of batteries for Internet of Things (IoT) applications. A new type of nitroxide-bearing organic radical polymers with polyphosphazene backbone (PPZ) was introduced recently ^[1]. PPZ polymers are stable, easy to synthesize and can be modified with a wide variety of side groups to control properties such as crystallinity, solubility and biodegradability. A theoretical capacity of 131 Ah kg⁻¹ has been reported for nitroxide-grafted PPZ polymers which makes them promising organic radical battery cathode candidates. To approach this capacity in real cells, the electron transfer within the cathode material must be optimized, which requires a fundamental understanding of the limiting factors of this process. Electron paramagnetic resonance (EPR) spectroscopy is a versatile tool for investigating electron transport in cathode materials. Its methods allow the measurement of spin densities, distinguishing between different interactions between spins and environment and, since EPR is non-invasive, studying redox processes in operando. Previous study ^[2] gave insight into radical distribution within the cathode and contact between active materials and conductive additive.

In this work, new TEMPO-grafted polyphosphazene and cyclotriphosphazene polymers are studied via EPR spectroscopy. Existence of spin clusters with high radical density, impenetrable by solvents, is observed in both, with estimated effective spin-spin relaxation time of less than 30 ns, which corresponds to strong interspin interactions. In such cases, experimental limitations prevent pulse EPR of radicals at high concentration or at room temperature. In order to overcome this challenge, longitudinal detection in EPR is discussed as method of investigation of electron transport in PPZbased organic cathodes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 47: Additive percolation and performance of polymer battery electrodes

Philip Zimmer^{a,b,c,d}, Christian Stolze^{a,b,c,d}, Kristin Schreyer^{a,b,c,d}, Martin D. Hage^{a,b,c,d}, Ulrich S. Schubert^{a,b,c,d}

^aHelmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

^bHelmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

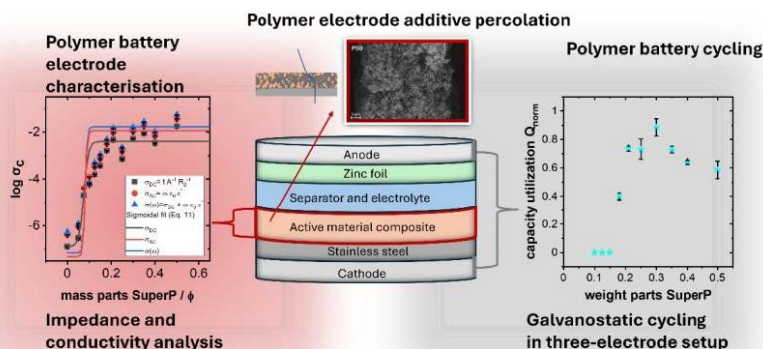
^cLaboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany

^dCenter for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, 07743 Jena, Germany

Composite electrodes for organic radical batteries (ORBs) combine an electronically dielectric TEMPO-bearing polymer with a conductive carbon additive, which is usually a carbon nanomaterial. In this investigation the spherical carbon black SuperP® (SP) is applied as conductive additive to enable charge transport within the polymer battery electrode. The generality of the structure-property relationships of the conductive additive percolation within the polymer composite electrode across different polymer battery systems is discussed regarding the relevance for the electrode formulation. This poster compares two full percolation investigations for an organic and aqueous polymer battery system, applying poly(2,2,6,6-tetramethyl-4-piperidinyl-N-oxyl methacrylate) (PTMA) with a carboxymethyl cellulose (CMC) binder on aluminum current collector, cycled in a non-aqueous ionic-liquid electrolyte,^[1] and poly(tetramethyl-4-piperidyl methacrylamide) (PTAm), an allaqueous-synthesized, acrylamide-based analogue, with a polyvinylidene fluoride (PVdF) binder on stainless steel, cycled against zinc as counter-electrode in an aqueous zinc perchlorate electrolyte. In both systems SP is used as additive and consequent analysis focus on the conductive properties of the composite mixtures. Dielectric spectroscopy, Nyquist plot - equivalent circuit evaluation, and distribution of relaxation times (DRT) identify a percolation transition of the SP phase within the composite polymer electrodes. The electronic percolation threshold is quite consistent between the two morphologies: 8.2–8.4 wt.-% SP for PTMA/CMC vs. 7.5–8.1 wt.-% SP for PTAm/PVdF, despite the differences in the morphology of the polymer, the polymers wettability, the polymer backbone and the applied binder. The DRT analysis further shows that, once percolated, both systems relax on a near-identical timescale ($\log \tau \approx -6.6$ to -6.8), consistent with SP-dominated conduction that is largely independent of the surrounding polymer matrix. Below the threshold, however, the two matrices differ in their direct-current conductivity (DC) derived from equivalent circuit fitting of the Nyquist plot: non-percolated PTAm electrodes exhibit a DC conductivity, of roughly 11 to 13 orders of magnitude higher than non-percolated PTMA electrodes, even though the conductivity, derived from the imaginary part of the permittivity of the pure polymer/binder phase in the percolation models is of comparable magnitude ($\sim 10^{-8} \text{ S m}^{-1}$) for

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both. This may point to differences in the conduction mechanism as PTAm shows a single, comparatively fast hopping-type relaxation ($\log \tau \approx -5.1$), against PTMA's slower, capacitively dominated charge-transfer response ($\log \tau \approx -3.5$ to -3.8). Galvanostatic cycling with potential limitation reveals where the two systems diverge most, while the electronic percolation threshold is quite in the same region, its translation into capacity utilization does not transfer similarly. PTMA electrodes saturate sharply to nearly 100% capacity utilization directly above the threshold and remain there up to the highest SP loadings tested. PTAm electrodes instead show a non-monotonic response, with capacity utilization peaking around 30 wt.-% SP before declining again at higher loadings, and the highest absolute discharge capacities shifting to 35 wt.-% SP – roughly twice the loading at which PTMA reaches its optimum, at around 15 wt.-%. This behavior may suggest that the electrode morphology and its performance is a non-monotonic function of additive content once increasing amounts of electrochemically inactive material may begin to block ion transport, and suggests that redox-center accessibility in PTAm electrodes is additionally limited by morphological factors – porosity, tortuosity, electrode thickness, and wettability – beyond electronic percolation alone.^[2] In the end, this investigation shows that the electronic percolation threshold of SP is a quite robust, transferable parameter that is largely insensitive to polymer chemistry and type of binder. Impedance spectroscopy is applied as a general characterization and pre-assembly screening tool for polymer battery electrode formulations. In contrast, the optimal SP loading for capacity utilization of the polymer batteries is system-specific and cannot be inferred from percolation threshold alone, underscoring the need to combine electrical percolation analysis with morphological and structural characterization when transferring electrode design rules between different organic battery chemistries.^[2]



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ABSTRACTS OF POSTER PRESENTATIONS

P 48: Spectroscopically probing radical association in viologen-based redox flow batteries

Pip Hendriks, G. A. Silva Testa, H. A. A. W. Elemans, E. W. Zhao

Radboud University

pip.hendriks@ru.nl

The electrochemical behaviour of redox-active organic molecules in redox flow batteries (RFBs) is often governed by intermolecular interactions that remain difficult to observe directly under realistic operating conditions. Viologens are particularly relevant in this context, as association between their reduced radical species can significantly alter their electrochemical and spectroscopic behaviour ^[1,2]. Methyl viologen (MV²⁺) provides a well-established model system for investigating these effects. Its one-electron reduction forms the radical cation MV^{•+}, which can be easily detected by Electron Paramagnetic Resonance (EPR) spectroscopy. At higher concentrations, MV^{•+} species can associate to form -dimers and related assemblies, which have completely different magnetic and optical properties than those of the free radical. In our previous work, operando benchtop EPR measurements of a methyl viologen (MV²⁺) RFB revealed substantially lower concentrations of detectable MV^{•+} than expected, suggesting that radical association plays an important role at even relatively low concentrations [3]. Here, we expand on that study by investigating the concentration-dependent behaviour of MV²⁺ using complementary operando benchtop EPR and UV-Vis spectroscopy. Both spectrometers are coupled to a flowing electrochemical system, enabling the electrolyte to be monitored continuously during reduction and oxidation. Operando EPR provides time-resolved information on the apparent concentration of MV[•] radicals, while UV-Vis spectroscopy follows changes in the absorption bands associated with the different electronic and associated states in solution. These preliminary results highlight how combined operando spectroscopic measurements can reveal molecular processes that are not accessible from electrochemical data alone. More broadly, this approach provides a framework for in

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ABSTRACTS OF POSTER PRESENTATIONS

P 49: Tracking Li⁺ association with redox-active molecules in the negolyte by mass spectrometry

Vasily Grebennikov, Jana Roithová^a, Evan Wenbo Zhao^b

^aSpectroscopy and Catalysis, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

^bMagnetic Resonance Research Center, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

vasily.grebennikov@ru.nl; jana.roithova@ru.nl; evanwenbo.zhao@ru.nl

Supporting-electrolyte ions are essential for charge transport in aqueous organic redox flow batteries (AORFBs), yet their molecular response to changes in redox-active species have rarely been observed in situ.^[1] Here, we used a previously developed flow-cell electrochemical electrospray ionisation mass spectrometry (EC-ESI-MS) approach to investigate the Li association with anthraquinone-2,7-disulfonate (AQDS), a commonly studied negolyte in AORFBs.^[2-4] Multi-step chronoamperometry coupled to continuous MS detection allowed the evolution of AQDS species to be followed as a function of applied potential. The results reveal Li-containing radical monomers together with dimeric and higher associated AQDS assemblies. These results reveal a potential-dependent and chemically heterogeneous distribution of Li-containing AQDS species, and highlight EC-ESI-MS as a powerful approach for resolving speciation in complex redox-active electrolytes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 50: Mechanistic understanding of lithium plating/stripping via cationic polymer coatings

Yuta Maeyoshi¹, Duy Anh Khuong¹, Fatimah Najirah Jumaah², Nur Atiqah Surib², Hikaru Sano¹, Mitsunori Kitta¹, Masahiro Yoshizawa-Fujita²

¹Research Institute of Electrochemical Energy, Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577, Japan

²Department of Materials & Life Sciences, Sophia University, 7-1 Kioi-cho, Chiyoda-ku, Tokyo 102-8554, Japan

y.maeyoshi@aist.go.jp

Lithium metal is a promising anode material for next-generation rechargeable batteries due to its high theoretical capacity (3860 mAh g⁻¹) and low electrochemical potential (-3.04 V vs. standard hydrogen electrode). However, its practical application is hindered by the growth of whisker-like Li (so-called Li dendrites) and continuous reductive decomposition of electrolytes. Polymers have attracted considerable interest as functional interfacial materials owing to their tunable structures and physicochemical properties ^[1]. In particular, cationic polymer coatings have been reported to control Li deposition morphology and improve the electrochemical performance of Li metal anodes ^[2]. However, the underlying mechanism remains unclear.

In this study, we employed poly(diallyldimethylammonium) (PDADMA)-based cationic polymers as model interfacial layers to understand the mechanism. We studied the mechanism of Li plating/stripping via PDADMA-based polymer coatings by electrochemical measurements and our recently developed operando microscopy with a transparent ultra-thin copper electrode ^[3]. Our operando microscopy revealed that the PDADMA-based polymer coating forms dense Li deposits and suppresses dead Li formation. These findings provide mechanistic insight into how cationic polymer coatings regulate Li plating/stripping and offer design principles for organic interfacial materials for Li metal anodes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 51: Dual-responsive organo-sulfur network cathodes for stable high-capacity polymer batteries

Ayda Gholamhosseini¹, Michael Walter¹

¹Freiburg Center for Interactive Materials and Bioinspired Technologies (FIT), University of Freiburg, Georges-Köhler-Allee 105, 79110 Freiburg, Germany

Lithium–sulfur (Li–S) batteries are promising candidates for energy storage systems due to having a high theoretical capacity (1675 mAh/g) ^[4,3], but also face some challenges, such as the polysulfide shuttle effect, which causes the battery capacity to decrease during charge and discharge cycling. There are different approaches to overcoming these challenges ^[5], one way is to covalently bond sulfur chains to organic structures ^[5,6] such as Naphthalene Diimide (NDI), and N-methylpyrrolidone (NMP). This covalent C–S bonding not only anchors sulfur, reduces the shuttle effect, but also provides additional redox-active sites from the organic backbone. Furthermore, by controlling the sulfur chain length through inverse vulcanization, we can balance high capacity (longer chains) with improved cycling stability (shorter chains).

In the present study, to have a comprehensive picture of the electronic states, we simulate X-ray absorption spectroscopy (XAS), X-ray emission spectroscopy (XES), and resonant inelastic X-ray scattering (RIXS) with density functional theory (DFT) performed using the GPAW code ^[2,1]. XAS probes unoccupied electronic states, while α -XES corresponds to a core-to-core transition (S 2p $\rightarrow$

1s). In contrast, β -XES involves valence-to-core transitions and therefore provides information on occupied valence states and is more sensitive to the chemical environment ^[8]. XES spectra are usually measured in the non-resonant region at incident energies around 2800 eV ^[7,8], much higher than the sulfur K-edge absorption energy of about 2470 eV. In RIXS, the energy of incident and emitted photons is correlated, allowing us to study both occupied and unoccupied states, as well as provide information on sulfur species within complex chemical environments. We compare our simulations to X-ray spectroscopy measurements from our experimental collaborators.

Our calculations indicate that variations in the dihedral angle of the sulfur chains and changes in the S–S bond length lead to shifts in the core-excitation energies in the XAS spectra. This combined experimental–theoretical approach provides insight into structure–property relationships and supports the rational design of stable, high-capacity polymer-based cathodes for next-generation Li–S batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 52: Ionization potentials and electron affinities of active materials of organic batteries

Anton S. Nizovtsev^{1,2}, Doreen Mollenhauer^{1,2}

¹Institute for Technical and Environmental Chemistry, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

²Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstrasse 12-14, 07743 Jena, Germany

anton.nizovtsev@helmholtz-berlin.de; doreen.mollenhauer@helmholtz-berlin.de

The application of redox-active organic compounds in the energy conversion and storage has gained significant attention over recent decades ^[1]. However, the development of high-performance organic batteries depends heavily on the specific characteristics of the underlying redox-active materials. In particular, ionization potential (IP) and electron affinity (EA) represent two fundamentally important molecular properties that determine a compound's suitability as a battery active material. They are closely related to the positions of the frontier molecular orbital energy levels and influence a battery's operating voltage, redox potential, and stability window. Importantly, IPs and EAs of moderately sized chemical systems can be accurately predicted by using high-level electronic structure methods, such as explicitly correlated coupled cluster theory with singles, doubles, and perturbative triples, CCSD(T)-F12. Subsequent calibration of density functional theory (DFT) methods against reference IP and EA values allows less computationally demanding theoretical methods to be applied to larger systems without substantial loss of accuracy.

In the present contribution, we compare DFT results with available experimental data and high-accuracy CCSD(T)-F12 data to assess the performance of a range of exchange-correlation density functionals for the calculation of IPs and EAs across for four classes of redox-active compounds, including (i) carbonyl compounds, (ii) N- and (iii) S-containing compounds, and (iv) radicals. A promising DFT-based computational strategy capable of reproducing IP and EA reference values with a reasonable accuracy is proposed. The results obtained provide a basis for computationally efficient first-principles screening and design of organic batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 53: Data-driven stochastic 3D microstructure modeling and electrochemical modeling of polymer-based batteries

A. Yessim¹, B. Prifling², M. Osenberg³, M. Paulisch-Rinke³, L. F. Schröder², L. Fuchs², S. Weber², L. Dodell², P. Zimmer⁴, M. Hager⁴, U. S. Schubert⁴, I. Manke³, V. Schmidt², T. Carraro¹

¹Institute of Modelling and Computational Science, Applied Mathematics, Helmut-Schmidt-Universität der Bundeswehr Hamburg, 22043 Hamburg, Germany

²Institute of Stochastics, Ulm University, 89069 Ulm, Germany

³Institute of Applied Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

⁴Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), 07743 Jena, Germany

yessima@hsu-hh.de

Polymer-based batteries offer promising prospects for safe, sustainable, and fast-charging electrochemical energy storage. Their performance is strongly influenced by the three-dimensional microstructure of the electrodes, which governs electronic conductivity, ion transport, and ultimately accessible capacity. Understanding the relationships between electrode microstructure and electrochemical properties is therefore essential for targeted electrode optimization. In this contribution, data-driven stochastic 3D microstructure modeling and electrochemical modeling are combined to investigate polymer-based battery electrodes. The basis is high-resolution 3D image obtained by focused ion beam scanning electron microscopy. In particular, we present an approach for calibrating the parameters of the stochastic microstructure model via single 2D SEM images by generating a large number of virtual 3D microstructures and their corresponding SEM images via physics-based simulation. A convolutional neural network is then trained to predict parameter of the underlying three-dimensional stochastic microstructure model from the simulated 2D SEM image. Complementarily, a physics-based electrochemical model is applied to a polymer cathode system to investigate the influence of material parameters on cell performance and to gain insight into limiting processes during electrode operation. Together, these approaches contribute to a more systematic understanding of the relationships between electrode microstructure and electrochemical behavior, supporting future microstructure-informed optimization of polymer-based battery electrodes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 54: Prediction of thermal decomposition pathways in high-performance phthalonitrile resins

D. S. Stepaniuk, D. I. Poliakova, S. S. Nechausov, U. S. Schubert, B. A. Bulgakov, D. Mollenhauer

Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstrasse 12-14, 07743 Jena, Germany

Institute for Technical and Environmental Chemistry, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

daria.stepaniuk@helmholtz-berlin.de; doreen.mollenhauer@helmholtz-berlin.de

The development of sustainable high-performance thermosetting polymers requires a detailed understanding of the molecular mechanisms governing their thermal stability and degradation. In this work, density functional theory (DFT) calculations in Gaussian package^[1] were employed to investigate the thermodynamics of competing decomposition pathways in partially bio-based phthalonitrile resin precursors differing in linker structure and substitution pattern. Structure optimizations and vibrational frequency calculations were carried out to obtain reaction Gibbs free energies and enthalpies at 298 and 653 K, the latter representing the experimental relevant conditions. Several decomposition pathways initiated by homolytic bond cleavage were systematically examined. Comparison of the calculated reaction Gibbs free energies revealed that the relative thermodynamic favorability of the investigated pathways strongly depends on the molecular structure of the precursor. The calculations further demonstrated that modifications of the linker and substitution pattern significantly influence the energetic ordering of competing reaction pathways. Although increasing the temperature lowered the reaction Gibbs free energies, the energetic ordering of the investigated pathways remained unchanged. These findings provide atomistic insight into the relationship between chemical structure and thermal stability and help rationale the experimentally observed differences among the investigated resin precursors.

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ABSTRACTS OF POSTER PRESENTATIONS

P 55: Computational screening of functionalized anthraquinones for organic redox chemistry, energy storage, and electrochemical CO₂ capture

Diego Bitzenhofer Betolaza¹⁻³, Wenbo Dong¹⁻³, Aleksandr Zaichenko¹⁻³, Fabian Knötzsch^{1,2,4}, Tilmann J. Neubert³, Ulrich S. Schubert^{1,2,4}, Doreen Mollenhauer¹⁻³

¹Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstrasse 12-14, 07743 Jena, Germany

²Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

³Institute for Technical and Environmental Chemistry (ITUC), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

⁴Institute for Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany

diego.bitzenhofer_betolaza@helmholtz-berlin.de;
doreen.mollenhauer@helmholtz-berlin.de

Anthraquinones are promising redox-active organic materials for energy-storage applications because their reversible electron-transfer chemistry can be tuned through molecular functionalization, making them attractive candidates for organic batteries. In addition, their reduced forms can interact reversibly with CO₂, enabling electrochemically switchable CO₂ capture. However, rational molecular design requires an understanding of the interplay between redox potential, charge localisation, structural changes, and binding thermodynamics^[1]. Here, we present a computational investigation of anthraquinone and nine substituted anthraquinone monomers as precursors for redox-active polymers. The compounds include vinyl-, methacryl-, methacrylamide-, alkyl-, and sulfonate-functionalized anthraquinones. A multistep computational workflow combining conformational sampling with GFN2-xTB/ALPB and density functional theory at the B3LYP-D4(BJ)/def2-TZVP level of theory with the COSMO solvation model was implemented to determine thermodynamic properties and reduction potentials in aprotic media.^{[2][3]} Results show pronounced substituent effects on anthraquinone redox properties, with methacrylamide-sulfonate substitution shifting the redox potential by 0.3 V relative to unsubstituted anthraquinone. Structural analysis of the neutral, radical-anion, and dianion states shows systematic carbonyl bond elongation upon reduction, indicating increased electron density at the carbonyl groups. Overall, this study establishes structure–property relationships relevant to both organic batteries and electrochemical CO₂ capture and provides a transferable computational workflow for screening redox-active monomers and guiding molecular design in organic redox chemistry.

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ABSTRACTS OF POSTER PRESENTATIONS

P 56: Comparative DFT study of solvent co-intercalation into graphite anodes

Dmytro Dudariev, Doreen Mollenhauer

Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena),
Lessingstrasse 12-14, 07743 Jena, Germany

Institute for Technical and Environmental Chemistry, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

dmytro.dudariev@helmholtz-berlin.de; doreen.mollenhauer@helmholtz-berlin.de

Electrochemical solvent co-intercalation into graphite anodes bypasses the desolvation penalty associated with conventional alkali-ion batteries, enabling ultrafast charge-transfer kinetics and highly reversible cycling via an SEI-free interface ^[1]. Ternary graphite intercalation compound (t-GIC) models traditionally assumed a constant solvent-to-ion ratio. However, recent operando measurements revealed a dynamic “flood and replace” storage mechanism, wherein the graphite gallery is initially flooded with excess free solvent before the solvent is ejected at higher states of charge ^[2]. The quantum-chemical driving forces behind this solvent ejection, and the origin of the contrasting cycling behaviour of Na-diglyme and Li-diglyme systems, remain unclear at the atomic level.

In this work, we employ a computational framework combining semi-empirical conformational searches with density functional theory (DFT) to evaluate the thermodynamic landscape of solvent co-intercalation. We calculate the solvent ejection free energy as a function of intercalant concentration by modelling thermodynamic states ranging from dilute domains to fully packed stages. Following our group's established energy partitioning scheme ^[3], formation energies are decomposed into structural deformation and binding energy contributions.

Preliminary results indicate that solvent ejection is driven by severe mechanical strain at high intercalant concentrations, naturally limiting gallery expansion to the values observed experimentally. This framework provides a molecular-level description of the thermodynamic driving forces governing solvent co-intercalation and offers design principles for optimizing co-intercalation electrolytes for post-lithium batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 57: Modelling redox and electronic properties of organic cathode materials: A case study on phenothiazine copolymers

John Symon Dizon^{a,b,c}, Daniel Brandell^b, Moyses Araujo^{a,d}

^aDepartment of Engineering and Physics, Karlstad University, Karlstad, Sweden

^bDepartment of Chemistry – Ångström Laboratory, Uppsala University, Uppsala, Sweden

^cInstitute of Physics, College of Arts and Sciences, University of the Philippines Los Baños, Laguna, Philippines

^dMaterials Theory Division, Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

johnsymon.dizon@kemi.uu.se

Decades of work on organic cathode materials point to lower-impact, tunable options, and redox active center mixed polymers (RACMPs) offer modular redox centers and conjugation that can be functionalized for performance. We investigate the redox properties of phenothiazine -bithiophene (PTZ- BT) conjugated copolymer (P1a) ^[1] within the framework of DFT. Geometry optimizations, SCF, and frequency analyses employed 6-311G(d,p) basis set with PCM implicit solvation during optimization/SCF and SMD for vibrational free-energy corrections. LC- ω HPBE range-separated hybrid (RSH) functionals were tuned per repeat unit with optimized α and β applied across calculations ^[2]. Each P1a oligomer (up to $n=7$ units) was incrementally oxidized from +1e to + n e. Oxidation potentials ϕ_{ox} computed from the optimally tuned RSH protocol show clear convergence toward the experimental value of ~ 0.20 V vs. Fc/Fc⁺, outperforming estimates from B3LYP and OHSE2PBE. NBO analysis indicates charge localization primarily on PTZ units with delocalization onto conjugating thiophene units. For $n>4$, structures converged upon oxidation to +5e. This suggests possible electrostatic repulsion of charges upon reaching a very high state of charge. These demonstrate that the tuned RSH/basis-set/solvation protocol reliably reproduces experimentally observed redox behavior of the copolymer. We now extend this towards obtaining a representative bulk polymer through classical MD evaporation, after which sequential quantum mechanics/molecular mechanics (s-QM/MM) calculations are done to evaluate potentials and electronic structure ^[3]. This multiscale modelling framework will allow us to assess how structural disorder and local environment effects influence the redox and electronic properties of RACMP-like systems.

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ABSTRACTS OF POSTER PRESENTATIONS

P 58: Validated process model for capacity fade prediction in a viologen–ferrocyanide flow battery

Juraj Volešín, Petr Mazúr, Alexandr Zubov, Jan Svoboda

University of Chemistry and Technology, Prague

volesinj@vscht.cz

The growing share of intermittent renewables makes reliable stationary energy storage increasingly important. Aqueous organic redox flow batteries (AORFBs) are one of many candidates. Their long-term deployment, however, is limited by several factors: chemical and electrochemical instability, membrane crossover, and limited energy density. We present a process model of an AORFB based on a 1,1'-bis(3-sulfonatopropyl)-4,4'-bipyridinium ((SPr)2V) negolyte and a ferrocyanide posolyte, developed as a tool for optimization of operating parameters and evaluation of mitigation strategies.

The model uses a 0D lumped-parameter formulation with four compartments (two tanks and two half-cells) separated by a cation-exchange membrane, described by 36 coupled ODEs ^[1]. It resolves cycling dynamics, redox-active species crossover, water transport, self-discharge, and the chemical degradation of the reduced (SPr)2V radical cation. Kinetic and water-transport parameters were estimated from mid-term cycling data, and the model was validated against cycling experiments for non-mixed and mixed electrolyte configurations. In the non-mixed configuration, each tank holds only its own active species. In the mixed configuration both are dissolved in both tanks, removing the gradient that drives net crossover.

Applied over 500 cycles, the model shows configuration dependence. In the non-mixed configuration, capacity utilization falls from 87% to 45%, driven mainly by species crossover and a 50% loss of negolyte volume. By contrast, in the mixed configuration, it declines from 78% to 60%, limited primarily by chemical degradation. Both maintain near-100% coulombic efficiency. Beyond this system, the same framework can be extended toward stack-level design optimization and, after re-parametrization of the kinetic and degradation submodels, transferred to other RFB chemistries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 59: Molecular simulation of TEMPO-substituted polyphosphazene in the context of organic radical batteries

Laura Hölzer¹, Diddo Diddens²

¹Institut für physikalische Chemie, Universität Münster, Corrensstraße 28-30, 48149 Münster, Germany

²Helmholtz Institute Münster (IMD-4), Forschungszentrum Jülich GmbH, 48149 Münster, Germany

lhoelzer@uni-muenster.de

Organic radical polymers are used as a redox-active cathode material in organic batteries. These organic radical batteries are seen as an alternative to traditional lithium-ion batteries due to their fast charge and discharge processes, and mechanical flexibility. For their application in the Internet of Things also high power densities and therefore good charge transport in the material are essential. One example for such an organic radical polymer is TEMPO-substituted polyphosphazene (PPZ). This polymer is of interest due to its high theoretical capacity and the high flexibility of the polymer backbone, which could possibly aid the charge transport in the material. Here PPZ is investigated using classical molecular dynamics simulations with the goal to guide further optimization of the material. The structure of the bulk material such as distances between the monomers and dwell times are analysed. Another property that is studied is the mobility of the anions. Furthermore the influence of different charge states of the polymer chains and the addition of solvent is considered.

ABSTRACTS OF POSTER PRESENTATIONS

P 60: High-throughput screening of molecular solar-thermal energy storage with a near-DFT machine-learned potential

Shuangjie Zhao, Doreen Mollenhauer

Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena);
Friedrich Schiller University Jena; Helmholtz-Zentrum Berlin

shuangjie.zhao@helmholtz-berlin.de; doreen.mollenhauer@helmholtz-berlin.de

Molecular solar-thermal (MOST) systems store energy in a metastable photoisomer, and the design tension mirrors organic batteries: raise the storage density without losing the kinetic stability that keeps the energy stored. In azobenzenes, light converts the planar E isomer into the metastable Z isomer; thermal Z→E back-isomerization releases the stored energy as heat. Usefulness hinges on the storage enthalpy H and the back-isomerization barrier E_a , which sets the lifetime: assuming comparable prefactors, ~ 1.4 kcal/mol more in E_a gives roughly tenfold longer storage^[1].

However, screening at the DFT level requires a conformer search, both isomer minima, and two reaction-path-verified transition states for each molecule. The rotational saddle point is an open-shell singlet diradical requiring broken-symmetry DFT. This workflow cannot be applied to thousands of candidates due to the significant computational cost. We therefore fine-tuned a foundation machine-learned interatomic potential: MACE-OMol-0- χ ^[2,3] showed the lowest zero-shot transition-state force error among eight benchmarked models and was fine-tuned as a committee of four models on 23,000 DFT structures from 30 molecules.

On 12 held-out molecules, the committee reproduces the lifetime-determining barrier with a mean absolute error of 0.87 kcal/mol and correctly identifies the dominant pathway. We then applied the model to jointly screen 4,969 candidates for ΔH and E_a , identifying a small subset that satisfies both storage-density and kinetic stability criteria.

A new molecule within the applicability domain can be evaluated in seconds. The workflow (DFT reference chain, fine-tuning, committee, active learning) is mechanism-agnostic and provides a general strategy for accelerating the screening of molecular energy storage materials and can potentially be transferred to redox-active organic electrode materials.

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ABSTRACTS OF POSTER PRESENTATIONS

P 61: Development of novel redox-active polymers based on benzimidazole, benzoxazole and benzothiazole – a combined theoretical and experimental screening approach

Wenbo Dong, Xhesilda Fataj, Martin D. Hager, Ulrich S. Schubert, Doreen Mollenhauer

Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstrasse 12-14, 07743 Jena, Germany.

Institute for Technical and Environmental Chemistry, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany.

wenbo.dong@helmholtz-berlin.de; doreen.mollenhauer@helmholtz-berlin.de

Organic redox-active polymers are promising materials for sustainable energy storage, but their electrochemical properties strongly depend on both their molecular structure and their local environment ^[1]. Here, computational screening and molecular dynamics simulations are combined with synthesis and electrochemical characterization to investigate benzimidazole-, benzoxazole-, and benzothiazole-based redox-active materials. The theoretical work consists of two complementary parts. First, a DFT-based screening workflow ^[2] is applied to a series of substituted redox-active model compounds. Conformer searches are followed by DFT calculations and redox-potential predictions to evaluate how different substituents and substitution patterns affect the electrochemical properties. The calculated trends are used to establish structure-property relationships and to support the selection of promising candidates for experimental investigation. Second, classical molecular dynamics simulations are used to study the influence of the molecular environment on the redox-active species, with particular focus on counterion interactions and solvation. The simulations show transient association between the counterion and the charged polymer site while retaining substantial ion mobility in acetonitrile. Selected systems will subsequently be investigated by ab initio molecular dynamics to provide a more detailed description of these interactions. Together with synthesis, electrochemical measurements, polymer preparation, and cell testing ^[3], these calculations provide complementary information on both intrinsic molecular properties and environmental effects. The combined approach supports the development of redox-active polymers with suitable properties for polymer-based batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 62: Rechargeable battery reaction mechanisms of trioxotriangulene crystal investigated by density functional theory calculations

Yukichika Kitano¹, Kohei Tada¹, Takashi Kawakami², Ryohei Kishi¹, Yasutaka Kitagawa¹

¹Graduate School of Engineering Science, The University of Osaka, Toyonaka, Osaka, Japan

²Graduate School of Science, The University of Osaka, Toyonaka, Osaka, Japan
u130411b@ecs.osaka-u.ac.jp

The battery system plays an important role as an energy source from wearable devices to energy storage systems. The use of battery systems is expanding more and more, and we should develop them with high energy density to meet the demands. Organic cathode materials (OCs) are promising candidates for high-energy-density battery systems. OC materials are lightweight and do not include transition metal elements; hence, the battery with OC will achieve not only high energy density but also a ubiquitous system. However, OC materials rapidly degrade through dissolution into the electrolytes during the charge/discharge cycle. For the molecular structural strategy, understanding the reaction mechanisms and crystallographic characteristics of high-durability and large-capacity OC materials is needed.

We then focused on tribromotrioxotriangulene (Br₃TOT) because the molecule exhibits high charge/discharge cycle stability.^[1] To establish a new molecular design concept for OC materials with high durability and large capacity, we performed density functional theory calculations on Li insertion into the Br₃TOT crystal and investigated the reaction mechanisms in detail. The calculation results showed that the Br₃TOT crystal accommodates Li atoms through the coordination mechanism followed by the intercalation mechanism. These results suggest that coordination and intercalation achieved high durability and large capacity, respectively.^[2]

In the presentation, we will talk about the Li insertion mechanism of Br₃TOT cathode materials with its crystal structural changes. In addition, we will discuss the Li insertion process in other trioxotriangulene derivatives: hydride derivative (H₃TOT), tri-tert-butyl derivative (tBu₃TOT), and trichloro derivative (Cl₃TOT). We will also discuss a virtual crystal of H₃TOT that has the same molecular arrangement as the Br₃TOT crystal (vir-H₃TOT), to investigate crystal-structure and substituent effects.

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ABSTRACTS OF POSTER PRESENTATIONS

P 63: First-principles study towards electronic band-structure engineering of organic cathode materials: From intermolecular band conduction to radical bands

Kohei Tada¹, Yukichika Kitano¹, Ryohei Kishi¹, Yasutaka Kitagawa¹

¹Graduate School of Engineering Science, University of Osaka, Toyonaka, Osaka, Japan

tada.kohei.es@osaka-u.ac.jp

First-principles electronic band-structure calculations based on density functional theory (DFT) are widely used to elucidate and predict the properties of inorganic materials such as oxides and sulphides. Theoretical investigations of charge-carrier diffusions, local atomic structures, and electronic states governing electrode potentials and diffusion barriers complement experimental studies, and in recent years, data-driven approaches combined with informatics has also been conducted. However, applications of these methods to organic cathode materials remain limited. One major reason is that charge/discharge processes induce changes in intermolecular interactions and localized radical states, making electronic band structures difficult to describe accurately. In this presentation, we discuss the importance of electronic band-structure calculations^[1] for the *in silico* design of organic cathode materials and introduce recent advances in computational methods^[2] together with representative applications^[e.g., 3]. In Ref. ^[1], the band structure of Li-inserted crystals of 5,6-dihydroxy-1,4-naphthoquinone was calculated using the hybrid-DFT method, and a comparison with experimental results clearly demonstrated band conduction arising from intermolecular interactions between organic molecules. In Ref. ^[2], we developed a computational method for analysing the radical bands generated during the charge/discharge processes of organic cathodes. Furthermore, Ref. ^[3] suggested that the radical band in trioxotriangulene contributes to improving its durability during battery operation. The presentation will also include additional application examples involving other functional organic molecules.

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ABSTRACTS OF POSTER PRESENTATIONS

P 64: Improving cycling stability of anthraquinone electrodes using a cellophane membrane

Saki Fukuma¹, Ryota Akai¹, Hikaru Sano¹, Masaru Yao¹

¹National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577, Japan

fukuma.s@aist.go.jp

Organic rechargeable batteries have attracted attention because of their high theoretical capacities and abundant organic resources. However, the dissolution of active materials into electrolyte solutions remains a major challenge for many lowmolecular-weight organic electrode materials. Anthraquinone (AQ) (Figure. a) is susceptible to such degradation, as dissolved AQ species can migrate to the lithium-metal electrode and contribute to capacity fading. We have previously improved the cycling performance of organic batteries by suppressing active-material dissolution, including the use of molecular additives ^[1] and oligomerization of active materials ^[2]. We also reported that solid electrolytes can suppress degradation by preventing the migration of dissolved active materials ^[3]. This finding suggests that controlling the migration of dissolved species is effective even when dissolution occurs. To apply this concept using a simpler separator-based approach, we investigated the use of a cellophane membrane. A cellophane membrane was introduced as a semipermeable separator to limit the migration of dissolved AQ species while maintaining lithium-ion transport. To evaluate its effectiveness, AQ/Li half-cells were assembled using either a cellophane membrane or a conventional separator, and their cycling performance was compared. After 100 cycles, the cell containing the cellophane membrane retained 26% of its initial discharge capacity, whereas the cell with the conventional separator retained only 4.3% (Figure. b, c). These results suggest that the improved capacity retention is associated with the suppressed migration of dissolved AQ species to the lithium-metal electrode by the cellophane membrane. This work highlights the potential of low-cost cellulose membranes as separator materials for improving the cycling stability of organic rechargeable batteries.

ABSTRACTS OF POSTER PRESENTATIONS

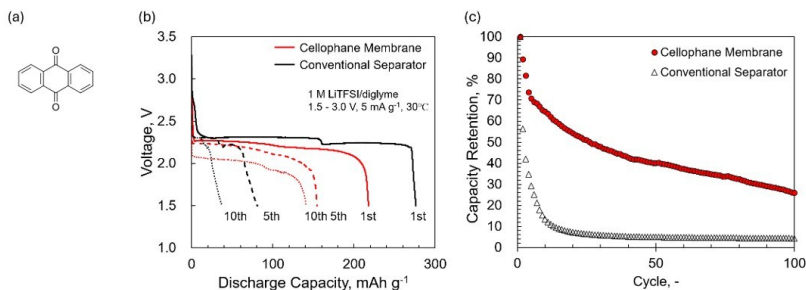


Figure. (a) Molecular structure of anthraquinone (AQ). (b) Discharge curves of AQ/Li half-cells with a cellophane membrane (red) and a conventional separator (black). (c) Capacity retention relative to the initial discharge capacity.

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ABSTRACTS OF POSTER PRESENTATIONS

P 65: Low-cost porous separators unlock practical aqueous biphasic redox flow batteries

Vikram Singh¹, Giu A. Silva Testa², Paula Navalpotro¹, Ruben Rubio-Presa³, Edgar Ventosa³, Evan Wenbo Zhao², Rebeca Marcilla^{1*}

¹Unit of Electrochemical Processes, IMDEA Energy Institute, Avda. Ramón de La Sagra 3, 28935 Móstoles, Madrid, Spain

²Magnetic Resonance Research Center, Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands

³Department of Chemistry, University of Burgos, Pza. Misael Bañuelos s/n, E-09001 Burgos, Spain

rebeca.marcilla@energia.imdea.org

Aqueous biphasic electrolytes (ABEs) suppress active-species crossover in redox flow batteries (RFBs) through thermodynamic phase separation, avoiding costly ion-exchange membranes.^[1,2] However, their use has largely been restricted to reactors with widely spaced electrodes, causing high resistance and low power density. Here, we demonstrate a zero-gap filter-press ABE RFB using a low-cost porous separator that electronically isolates the electrodes while preserving the liquid-liquid interface, enabling efficient ion transport and compatibility with conventional cell designs. Separator pore size governs crossover, self-discharge, and long-term performance. The optimized separator achieves coulombic efficiencies above 99%, stable cycling for up to 1000 cycles, high active-material concentrations, and superior peak power densities relative membrane-less ABE. It outperforms conventional porous polyolefin separators under biphasic conditions and approaches Nafion performance at substantially lower cost. Operando NMR, UV-vis-NIR spectroscopy, EPR, and in-line pH monitoring reveal viologen redox speciation and interfacial chemistry. UV-vis-NIR identifies radical-ion-associated species, whereas attenuation of the EPR signal indicates depletion of free radicals through association. Molecular dynamics simulations of the ABE and 1 M KCl electrolytes complement these observations by describing phase organization and dimer or higher-order aggregate formation. The biphasic environment promotes radical association, suppresses parasitic reactions and self-discharge, and maintains near-neutral pH. These results establish porous cellulose separators as a practical, economical route to zero-gap ABE RFBs.

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ABSTRACTS OF POSTER PRESENTATIONS

P 66: Stabilizing lithium anode interfaces via in-situ PEGDA polymerization for high-voltage lithium metal batteries

Vikram Raghuraman^{a,b,c}, Tobias Arlt^a, Qingping Wu^{a*}, Yan Lu^{a,b,c*}

^aInstitute of Electrochemical Energy Storage, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

^bHelmholtz Institute for Polymers in Energy Applications Jena, Lessingstrasse 12-14, 07743 Jena, Germany

^cInstitute for Technical and Environmental Chemistry, Friedrich Schiller University Jena, Philosophenweg, Jena, Germany

yan.lu@helmholtz-berlin.de; qingping.wu@helmholtz-berlin.de

The pursuit of high-energy-density batteries has revitalized interest in Lithium (Li) metal anodes. However, the commercialization of Li-metal batteries is bottlenecked by the stochastic growth of Li-needles (dendrites) and the continuous consumption of electrolyte at the reactive interface. While liquid electrolytes (LE) offer high conductivity, they fail to provide the mechanical modulus required to suppress this needle-like growth ^[1]. To stabilize the lithium anode interface, we investigate an in-situ polymerized Poly (ethylene glycol) diacrylate (PEGDA) electrolyte with in Ethylene Carbonate (EC), Dimethylene Carbonate (DMC), and Fluoroethylene carbonate (FEC), which offers a promising middle ground by ensuring conformal contact with the electrode before cross-linking into a supportive matrix ^[2]. The FEC is critical as it forms a Fluorine-rich Solid Electrolyte Interphase (SEI) that is chemically stable against Lithium and forms a gap-free interface of very low resistance ^[3]. The resulting integrated polymer electrolyte (PEGDA-10 IPE) successfully forms a robust, LiF-rich SEI directly on the Li metal anode surface and exhibits a high oxidative stability up to 4.8 V and delivers a stable, long-term cycling exceeding 700 hours at 0.5 mA cm⁻². Furthermore, scanning electron microscopy confirms a uniform, Li globular morphology, demonstrating the system's ability to effectively mitigate detrimental Li-needle propagation for highly stable lithium metal batteries.

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ABSTRACTS OF POSTER PRESENTATIONS

P 67: Anion-exchange-enabled hydrogel electrolytes with high Zn²⁺ transference for dendrite-free flexible zinc-ion batteries

Jung Woo Hong¹, Yeon Su Kim¹, Zuyang Hu¹, Hyungyu Cho¹, Gun Jang¹, Minjun Hwang¹, Hye Rin Park¹, Jun Su Kim¹, Ho Seok Park^{1,2,3,4}

¹School of Chemical Engineering, Sungkyunkwan University, Suwon, Republic of Korea

²SKKU Institute of Energy Science and Technology (SIEST), Sungkyunkwan University, Suwon, Republic of Korea

³SKKU Advanced Institute of Nano Technology (SAINT), Sungkyunkwan University, Suwon, Republic of Korea

⁴Department of Health Sciences and Technology, Samsung Advanced Institute for Health Sciences and Technology (SAIHST), Sungkyunkwan University, Suwon, Republic of Korea

dannykim98@skku.edu

Flexible aqueous zinc-ion batteries (ZIBs) are attractive for wearable and implantable energy storage owing to their high safety, low cost, and mechanical compliance ^[1]. However, conventional hydrogel electrolytes suffer from unregulated anion mobility, which triggers concentration polarization, dendrite growth, and parasitic reactions. Single-ion-conducting designs promise near-unity transference ^[2] but remain difficult to realize in aqueous ZIBs. Herein, we report a high-Zn²⁺-transference hydrogel electrolyte (ex-PDADAM) prepared by exchanging Cl⁻ with ClO₄⁻ at quaternary ammonium (NR₄⁺) sites within a poly(diallyldimethylammonium)-polyacrylamide co-network. This single anion-exchange step fulfills three functions at once: (i) electrostatic immobilization of anions suppresses anion migration and raises the Zn²⁺ transference number to 0.86; (ii) multivalent ionic crosslinks between NR₄⁺ and ClO₄⁻ reinforce the network toughness to 51.25 MJ m⁻³; and (iii) restructuring of the confined-water hydrogen-bonding network widens the electrochemical stability window to 2.75 V. The strong ClO₄⁻-NR₄⁺ binding arises from electrostatic attraction combined with unconventional C-H...O hydrogen bonding ^[3]. The ex-PDADAM hydrogel delivers an ionic conductivity of 8.10 mS cm⁻¹ at 25 °C, enabling Zn||Zn symmetric cells to cycle stably for over 2000 h at 1 mA cm⁻² (35 mV overpotential). Flexible 4 × 3 cm² pouch cells paired with vanadium-oxide cathodes deliver ~270 mAh g⁻¹ under 0°-360° bending and retain 90.9% capacity after 300 cycles. This work establishes anion-exchange chemistry as a versatile strategy toward mechanically robust, high-transference hydrogel electrolytes for flexible ZIBs.

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ABSTRACTS OF POSTER PRESENTATIONS

P 68: Process-structure-property relationships in porous cation-exchange membranes for alkaline redox flow batteries

Andrea Diaz¹, Zhongbo Zhang^{1,2}, Samantha Alderden¹, Mincheol Kim¹, Zhiguang Li², Lu Zhang², Shrayesh Patel^{1,2}

¹Pritzker School of Molecular Engineering, University of Chicago

²Argonne National Laboratory

andreadiaz@uchicago.edu

Aqueous organic redox flow batteries are promising candidates for large-scale energy storage because of their modular design and the structural tunability of organic redox-active materials ^[1]. Their performance and lifetime, however, depend strongly on the membrane that separates the electrolytes containing redox-active species. Effective membranes must balance promoting ionic transport with blocking redox-active species crossover while remaining chemically stable and economically scalable ^[2].

Here, we investigate process -structure -property relationships in porous cation-exchange membranes prepared from engineering polymer feedstocks using nonsolvent-induced phase separation ^[3] followed by chemical functionalization. Membrane fabrication and post-processing conditions are systematically varied to understand how processing influences membrane morphology, ion-exchange characteristics, ionic resistance, permeability, and electrochemical performance.

The membranes are evaluated using complementary structural, physicochemical, and electrochemical characterization methods, including scanning electron microscopy, electrochemical impedance spectroscopy, ion-exchange capacity measurements, permeability testing, and redox flow battery cycling. This work demonstrates how membrane transport properties can be tuned through processing and functionalization and provides design considerations for the development of scalable, lower-cost ion-selective membranes for aqueous organic redox flow battery systems.

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ABSTRACTS OF POSTER PRESENTATIONS

P 69: Electrolyte confinement in COFs: How does nanopore structure control the solvent distribution in Li-S cathodes?

Andreas Döll¹, Sébastien Groh¹, Jin Yang², Joachim Dzubiella¹

¹Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder Straße 3, D-79104 Freiburg, Germany

²Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstr. 12-14, 07743 Jena, Germany

andreas.doell@physik.uni-freiburg.de

Lithium-sulfur (Li-S)-based batteries exhibit high theoretical energy density, which could provide the basis for novel energy storage technology. However, several obstacles still challenge the performance of this innovative battery concept, such as slow ion kinetics and the polysulfide-shuttle effect. Covalent organic frameworks (COFs) as Li-S cathode materials have emerged as possible candidates to combat these issues. COFs are chemically stable against the electrolyte and offer well-defined ion diffusion pathways due to their highly ordered porous structure, promoting diffusion. Notably, the shuttle effect can be suppressed in COF cathodes through direct incorporation of sulfur. Here, we report the structural properties of 2D vinylene-linked COFs using bromine to anchor sulfur (VCOF-Br). We investigate two VCOF-Br structures with distinct pore sizes and explore their characteristics via classical non-reactive molecular dynamics simulations. A force field for VCOF-Br was developed and validated by comparing the simulated XRD pattern to experimental measurements and matching the energetic landscape of molecular statics to density functional theory calculations. Furthermore, the simulations shed light on the interaction of the VCOF-Br with DME/DOL-based electrolyte containing LiTFSI. Our data reveals that electrolyte confinement results in highly ordered solvent structures in the pores, manifested by pronounced and localized accumulation. In particular, DME organizes in a ladder-like fashion from layer to layer, exhibiting an order parameter close to unity at the wall, whereas DOL preserves its rotational degrees of freedom. These simulations provide insight into ordered solvent structures in COF pores, which can have significant implications for salt uptake of the system.

ABSTRACTS OF POSTER PRESENTATIONS

P 70: Towards bulk liquid redox-active organic materials for energy storage

Angelina Castro Trujillo, R. B. Jethwa, I. Stepanenko, Stefan A. Freunberger

Institute of Science and Technology Austria

Angelina.CastroTrujillo@ist.ac.at

Redox-Active Organic Materials (ROMs) emerged as a promising alternative to current battery technologies to meet the needs in sustainability, elemental abundance, low-cost production, and recyclability. However, their implementation in batteries remains a challenge, as achieving high energy densities requires high concentrations of ROMs. Moreover, at high concentrations, limitations related to charge transport, solubility, phase behavior, and material utilization become crucial. In solid-state systems, achieving energy densities competitive with current Lithium-ion batteries is limited by the poor charge transport in solid ROMs, requiring dilution with large amounts of conductive carbon additives.^[1] In redox flow batteries (RFBs), increasing the volumetric energy density remains a topical challenge given otherwise prohibitive system costs.^[2] Therefore, understanding the limiting processes and properties of ROMs at high concentrations is essential to overcome those limitations.^[3]

Herein, we explore the behavior of ROMs in highly concentrated systems to understand how concentration and state of charge influence their physicochemical properties. We study known moieties, which have not been investigated in their bulk liquid state, and we introduce new classes of n- and p-type molecules. The oxidized states of p-type ROMs were synthesized with different counter ions (bis(trifluoromethanesulfonyl)imide [TFSI⁻], and tetrafluoroborate [BF₄⁻]). The physicochemical properties across the state of charge, including solubility, phase behavior, viscosity, conductivity, chemical stability, and reversibility, were systematically analyzed and compared. Our results highlight that exploiting the full potential of ROMs requires understanding limiting processes across the full state of charge, given that major changes occur between discharged and charged states.

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ABSTRACTS OF POSTER PRESENTATIONS

P 71: Scaling up membrane-less redox flow batteries using aqueous biphasic electrolyte

Karim Boutamine*, Camiel Kroonen**, Elsa Musy, Alexandra Lyons, Felix Heiland, Alexandre Crocetti, Soumyadeep Paul, Anetta Platek-Mielczarek

Unbound Potential AG, Bönirainstrasse 14/16, 8800 Thalwil, Switzerland

<https://www.unbound-potential.com/>

* k.boutamine@unbound-potential.com; ** c.kroonen@unbound-potential.com

Redox flow batteries (RFBs) are promising technology for long-duration energy storage because their power and energy capacity can be scaled independently. Most conventional RFB architectures use ion-selective membranes to separate the electrolyte while enabling ionic transport. However, these membranes contribute to system cost, electrical resistance, design complexity, and durability limitations. In addition, the cost and price volatility of vanadium electrolyte remain barriers to the broader deployment of conventional vanadium RFBs. These challenges have motivated the development of aqueous organic electrolytes based on potentially scalable raw materials and supply chains.

At Unbound Potential we rethink the cell architecture to enable the use of aqueous-organic electrolyte without the need to use membranes. The system uses an aqueous biphasic electrolyte in which two liquids are formed through the salting-out effect (top and bottom phase, TP and BP respectively). The resulting liquid-liquid interface provides separation of the redox-active species without requiring a solid ion-selective membrane (membrane-less architecture). Under the investigated operating conditions, the electrolyte exhibits an ionic conductivity min. 80 mS cm^{-1} , with a viscosity of 3-5 mPa·s.

In this work, we present the scale-up of this architecture to a 10-cell stack with an active electrode area of 500 cm^2 per cell and more than 5 L of electrolyte per half-cell, integrated into a fully automated prototype operating in a relevant operational environment (TRL5). At a current density of 10 mA cm^{-2} , the stack achieved a coulombic efficiency of 98%, a voltage efficiency of 77%, and an energy efficiency of 75%. The measured area-specific resistance was $4 \Omega \text{ cm}^2$, while the pressure drop across the stack was $<400 \text{ mbar}$ at an electrolyte flow rate of 6 L min^{-1} . The system maintained stable SOC for 450 cycles.

This work provides engineering insights into the scale-up of biphasic aqueous-organic RFBs and establishes design requirements for larger stacks and pilot-scale systems.

ABSTRACTS OF POSTER PRESENTATIONS

P 72: Scaling up membrane-less redox flow batteries using aqueous biphasic electrolyte

Karim Boutamine^{*}, Camiel Kroonen^{**}, Elsa Musy, Alexandra Lyons, Felix Heiland, Alexandre Crocetti, Soumyadeep Paul, Anetta Platek-Mielczarek

Unbound Potential AG, Bönirainstrasse 14/16, 8800 Thalwil, Switzerland

^{*} k.boutamine@unbound-potential.com; ^{**} c.kroonen@unbound-potential.com

Redox flow batteries (RFBs) are promising technology for long-duration energy storage because their power and energy capacity can be scaled independently. Most conventional RFB architectures use ion-selective membranes to separate the electrolyte while enabling ionic transport. However, these membranes contribute to system cost, electrical resistance, design complexity, and durability limitations. In addition, the cost and price volatility of vanadium electrolyte remain barriers to the broader deployment of conventional vanadium RFBs. These challenges have motivated the development of aqueous organic electrolytes based on potentially scalable raw materials and supply chains.

At Unbound Potential we rethink the cell architecture to enable the use of aqueous-organic electrolyte without the need to use membranes. The system uses an aqueous biphasic electrolyte in which two liquids are formed through the salting-out effect (top and bottom phase, TP and BP respectively). The resulting liquid-liquid interface provides separation of the redox-active species without requiring a solid ion-selective membrane (membrane-less architecture). Under the investigated operating conditions, the electrolyte exhibits an ionic conductivity min. 80 mS cm⁻¹, with a viscosity of 3-5 mPa·s.

In this work, we present the scale-up of this architecture to a 10-cell stack with an active electrode area of 500 cm² per cell and more than 5 L of electrolyte per half-cell, integrated into a fully automated prototype operating in a relevant operational environment (TRL5). At a current density of 10 mA cm⁻², the stack achieved a coulombic efficiency of 98%, a voltage efficiency of 77%, and an energy efficiency of 75%. The measured area-specific resistance was 4 Ω cm², while the pressure drop across the stack was <400 mbar at an electrolyte flow rate of 6 L min⁻¹. The system maintained stable SOC for 450 cycles.

This work provides engineering insights into the scale-up of biphasic aqueous-organic RFBs and establishes design requirements for larger stacks and pilot-scale systems.

ABSTRACTS OF POSTER PRESENTATIONS

P 73: Volumetric confinement underlies the role of SiO₂ in ionogel electrolytes

Ngoc Anh Ta^{1,3}, He Jia^{1,3*}, Yan Lu^{1,2,3*}

¹Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

²Institute of Electrochemical Energy Storage, Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

³ITUC, Friedrich Schiller University Jena

he.jia@helmholtz-berlin.de; yan.lu@helmholtz-berlin.de

Lithium-ion transport in polymer-based ionogel electrolytes is closely coupled to their complex coordination environment. Conventional strategies regulate Li⁺ transport mainly through electrolyte composition or molecular and network design. Here, using a poly(ionic liquid)/ionic liquid/lithium salt electrolyte containing SiO₂ nanoparticles as a model system, we reveal an underappreciated role of SiO₂ beyond mechanical reinforcement: volumetric confinement. SiO₂ reduces the accessible volume of the electrolyte, intensifying local interactions, reorganizing Li⁺ coordination, and constraining the collective redistribution of electrolyte components under applied voltage. A combination of structural and spectroscopic techniques, including SAXS, TEM, operando Raman spectroscopy, and FTIR spectroscopy, reveals the resulting confined architecture and associated changes in coordination. PFG-NMR further shows enhanced Li⁺ and ionic-liquid diffusion coefficients, demonstrating that confinement alters their transport dynamics. We attribute these effects to a confinement-regulated transport landscape with more defined migration pathways and suppressed polarization-induced redistribution. The resulting ionogel delivers an ionic conductivity around 1 mS cm⁻¹ at 20 °C and enables stable Li plating/stripping for over 3000 h at 0.2 mA cm⁻². These findings establish volumetric confinement as an important mechanism for regulating coordination and ion transport in ionogel electrolytes.

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ABSTRACTS OF POSTER PRESENTATIONS

P 74: Investigating an ionic liquid-based deep eutectic solvent for organic batteries

Sadeeda^a, Tim Beuter^a, Benjamin Schick^a, Philipp Schuster^b, Alexander Kuehne^b, Timo Jacob^{a,c,d}

^aInstitute of Electrochemistry, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany

^bInstitute of Organic and Macromolecular Chemistry, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

^cHelmholtz Institute Ulm (HIU) for Electrochemical Energy Storage, Helmholtz-str. 11, 89081 Ulm, Germany

^dKarlsruhe Institute of Technology (KIT), P.O. Box 3640, 76021 Karlsruhe, Germany

sadeeda@uni-ulm.de

Organic batteries offer a promising alternative to metal-ion energy storage, providing structural tunability, low-cost synthesis, and reduced reliance on scarce metals. Yet their performance is often limited not by electrode chemistry, but by electrolyte incompatibility leading to active material dissolution, poor ionic conductivity, and polymer degradation ^[1]. Ionic liquids offer a promising solution, with negligible volatility, wide electrochemical windows, and tunable cation-anion structures suited for organic redox-active materials ^[2]. However, many ionic liquids are highly viscous which limits ion mobility, lowers practical conductivity, and hampers rate performance which offsets their otherwise favorable stability and safety profile ^[2]. On the other hand, understanding of Deep Eutectic Solvents (DES) can provide valuable design insights by combining a hydrogen bond donor with an ionic liquid to circumvent the aforementioned limitations. Such DES can allow higher tunability, potentially leading to electrolytes suitable for organic redox chemistries, mitigating transport limitations while advancing cycling stability.

In this context, we have investigated a new DES system consisting of the ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide ([EMIm][TFSI]) and a hydrogen bond donor, N-methylacetamide (NMA). In the first step, differential scanning calorimetry was used to evaluate the corresponding phase

ABSTRACTS OF POSTER PRESENTATIONS

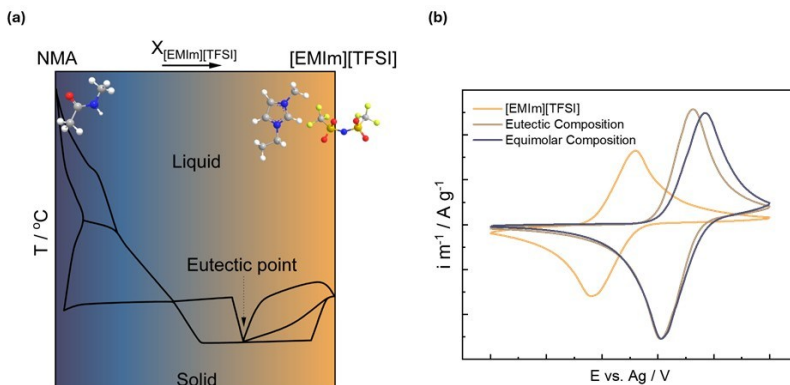


Figure 1: (a) Phase diagram of NMA – [EMIm][TFSI] exhibiting mixture of phases and the eutectic point marked, and (b) 100th cycle of cyclic voltammetry of pure [EMIm][TFSI], Eutectic composition and the equimolar composition.

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ABSTRACTS OF POSTER PRESENTATIONS

P 75: 3D-printable water-in-salt hydrogels for zinc-organic batteries

Sergey Nechausov^{a,b}, Martin Hager^{a,b,c}, Ulrich S. Schubert^{a,b,c}

^aHelmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstrasse 12-14, 07743 Jena, Germany

^bHelmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

^cLaboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, 07743 Jena, Germany

sergei.nechausov@hipole-jena.de

For next-generation sustainable energy storage, aqueous zinc-organic batteries are a promising candidate. In safe, environmentally friendly, and low-cost aqueous environments, they utilize metallic zinc anodes and organic cathodes. Rechargeable zinc batteries, however, are often hindered by zinc dendrite growth, which limits cycling stability. The water-in-salt electrolytes provide an effective method to suppress zinc dendrite formation and expand the electrolyte electrochemical stability window ^[1]. In this study, we developed 3D-printable, ionically conductive, and moisture-self-regulating water-in-salt hydrogel (WiSH) as electrolyte for zinc-organic battery electrodes. To enhance the stability of the WiSHs in air, a dual-salt strategy was employed: chaotropic Zn(ClO₄)₂ was added to disrupt the water structure and improve battery performance while hydrophilic ZnCl₂ was incorporated to utilize its deliquescent properties for maintaining self-regulated moisture content across a wide range of humidity and even after vacuum desiccation. Furthermore, we infused TEMPO-polymer-based cathode slurry into intricate 3D printed structures to increase ions availability for cathode material. This engineered architecture shortens the ion diffusion pathways and maximizes the electrochemically active surface area, facilitating redox kinetics and increasing organic redox active material utilization. In summary, these 3D-printed WiSHs enabled aqueous zinc-organic batteries to achieve high capacity and excellent cyclability, maintaining robust performance at low temperatures and under ambient air conditions.

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ABSTRACTS OF POSTER PRESENTATIONS

P 76: Charge-transfer complex with donor polymers containing hydroxy moieties for highly lithium-ion based solid electrolytes

Toshinori Kozakai, Akinari Chiba, Kenichi Oyaizu

Department of Applied Chemistry, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan

oyaizu@waseda.jp

Solid polymer electrolytes (SPEs) have attracted considerable attention for implementing the all-solid-state lithium batteries due to their good interfacial properties and processability. However, their low ionic conductivity remains a significant problem. This is because ions are trapped by the polymer chain in the conventional SPEs. To address this issue, our group has been focusing on SPEs with unconventional conduction mechanisms using charge-transfer complexes (CTCs) such as phenylene sulfide-based donor polymers and quinone acceptors ^[1]. Nevertheless, the factors governing high ionic conductivity in these CTC-based electrolytes are unclear.

Recent studies have shown that water enhances the ionic conductivity of charge-transfer complex (CTC)-based electrolytes, suggesting that hydroxy groups play an important role in ion transport ^[2]. However, low-molecularweight plasticizers such as water may compromise electrochemical stability ^[3]. Therefore, we aimed to achieve both high ionic conductivity and electrochemical stability by directly incorporating hydroxy groups into the donor polymer.

Specifically, in this study, hydroxy-functionalized poly(phenylene sulfide) (OHPPS) was employed as the donor polymer, and CTC-based solid polymer electrolytes with different OHPPS contents were prepared their ionic conductivities were evaluated. Ionic conductivity increased with increasing OHPPS content, reaching 2.1×10^{-4} S cm⁻¹ at 60 °C and remaining on the order of 10⁻⁴ S cm⁻¹ even at room temperature. Furthermore, the electrolyte exhibited oxidative stability up to 5.6 V vs. Li/Li⁺. These results demonstrate that incorporating hydroxy groups directly into CTCs is an effective strategy for achieving both high ionic conductivity and electrochemical stability.

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ABSTRACTS OF POSTER PRESENTATIONS

P 77: The influence of fluorine-free ionic liquids on the electrochemical behavior of PTMA cathodes for organic radical batteries

Xiao Yao^{a,b}, Christian Friebe^c, Ulrich S. Schubert^{a,d}, Andrea Balducci^{a,b}

^aCenter for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany

^bInstitute for Technical Chemistry and Environmental Chemistry, Friedrich Schiller University Jena, Jena, Germany

^cHelmholtz Institute for Polymers in Energy Application Jena (HIPOLE Jena), Jena, Germany

^dLaboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany

Poly(2,2,6,6-tetramethylpiperidiny-N-oxymethacrylate) (PTMA) is considered one of the most promising cathode materials for organic radical batteries. In this study, we report the use of the fluorine-free ionic liquid 1-butyl-2,3-dimethylimidazolium bis(oxalato)borate (BDMimBOB) as an electrolyte salt for PTMA-based electrochemical systems. The influence of the solvent selection was systematically investigated using acetonitrile (ACN), γ -butyrolactone (GBL) and γ -valerolactone (GVL).

The results of this study show that solvent selection plays a decisive role in determining both half-cell and hybrid device performance. Although ACN-based electrolyte displayed the highest ionic conductivity and allows the best rate capability, its negative impact on cycling stability limits its suitability for energy storage devices. In contrast, the use of GBL-based electrolyte allows good rate performance and excellent cycling stability (capacity retention of 98% after 500 cycles at 1C).

Based on these findings, hybrid devices containing PTMA-based positive electrode and activated carbon (AC)-based negative electrode were subsequently assembled using lactone-based electrolytes. Among the investigated devices, the GBL-based electrolyte delivered the best overall device performance, achieving energy density up to ca. 30 Wh kg⁻¹ over a power range of 7-300 W kg⁻¹ together with superior cycling stability after 500 cycles at 1C with capacity retention of 70%. These results show that 1.5 M BDMimBOB in GBL is a promising electrolyte for PTMA-based organic radical batteries and hybrid energy-storage devices.

ABSTRACTS OF POSTER PRESENTATIONS

P 78: Modulating phase behavior of micellar electrolytes for high-energy-density organic redox flow batteries

Youngsu Kim, Kisuk Kang*

Seoul National University

youngsufous@gmail.com

Achieving high solubility of redox-active organic molecules (ROMs) in organic redox flow batteries (RFBs) has relied on laborious functional group engineering that raises the material cost. ^[1] Micellar solubilization offers a non-covalent alternative, yet the accessible ROM concentration is limited by a phase transition to a viscous liquid crystalline phase at high surfactant concentration. ^[2] Herein, we identify inter-micelle electrostatic repulsion as the origin of this transition, and demonstrate that shortening the hydrophobic tail of the surfactant from cetyl- (CTAC) to octyltrimethylammonium chloride (OTAC) lowers the micelle surface charge density. The weakened repulsion delays the liquid crystal formation and extends the flowable micellar phase to higher volume fractions, increasing the maximum solubility of (2,2,6,6-tetramethylpiperidin-1-yl) oxyl (TEMPO) from 0.8 M to 1.2 M. Despite the higher micelle content, the catholyte maintains a comparable viscosity due to the diminished electroviscous effect, accompanied by an upshift in the redox potential. Harnessing these properties, a full flow cell employing the 9 m OTAC + 1.2 M TEMPO catholyte delivers a high energy density. This work uncovers the phase behavior that sets the upper limit of micellar solubilization, and offers surfactant molecular design as a versatile handle to push this limit, expanding the scope of non-covalent chemistry in organic RFBs.

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ABSTRACTS OF POSTER PRESENTATIONS

P 79: Hydroxy-group in improving ionic conductivity of sodium solid-polymer-electrolyte under polymer-in-salt

Yuki Ogawa, Akinari Chiba, Kenichi Oyaizu

Department of Applied Chemistry, Waseda University

oyaizu@waseda.jp

Although Li-ion batteries with high energy density are widely used in many electronic devices such as smartphones and electric vehicles, they use the rare and expensive element lithium as the cathode. To solve this problem, next-generation batteries like Na-ion batteries, which use inexpensive and abundant sodium, are attracting considerable attention. Moreover, solid-state electrolytes for the Na-ion batteries are insensibly studied to reduce the risks on electrolyte leakage and ignition, and to improve the energy density by laminating the electrodes and the electrolytes. Among them, solid polymer electrolytes (SPEs) are advantageous in flexibility and processability. However, their ionic conductivities are generally poor when compared to other candidates. This is because the ion conduction in the conventional SPEs is restricted by the segmental motion of the polymer chain.^[1] Thus, this problem is inherently difficult to solve.

We have previously demonstrated that ions are transported by an unconventional conduction mechanism involving the thermal motion of lithium salt in lithium-ion conductive SPEs under polymer-in-salt conditions, where a small amount of polymer is dissolved in an excess of salt.^[2] Inspired by this fact, we assumed that the ion transportability of Na-ion-conductive SPEs could also be improved using a similar approach. Specifically, in this research, SPEs containing polymers with hydroxyl groups, which are expected to promote salt dissociation through hydrogen bonding, were prepared and their ionic conductivities were evaluated.^[3] The SPEs exhibited a high conductivity exceeding 10^{-4} S/cm at 60 °C under polymer-in-salt conditions. The detailed conduction mechanisms will also be discussed in the presentation.

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ABSTRACTS OF POSTER PRESENTATIONS

P 80: PEG-crosslinked quaternized poly(phenylene oxide) anion exchange membranes for TMA-TEMPO/methyl viologen redox flow batteries

Mosayeb Gharakhloo^{1,2}, Mohammed Jamshid^{1,2}, Moritz Kunze^{1,2}, Koosha Ehtiati^{3,5}, Martin D. Hager^{1,2,3,4,5}, Felix H. Schacher^{1,2,3,4,5}, Ulrich S. Schubert^{1,2,3,4,5}

¹Helmholtz Institute for Polymers in Energy Applications Jena (HIPOLE Jena), Lessingstraße 12-14, 07743 Jena, Germany

²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany

³Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, 07743 Jena, Germany

⁴Jena Center for Soft Matter (JCSM), Friedrich Schiller University Jena, Philosophenweg 7, 07743 Jena, Germany

⁵Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany

mosayeb.gharakhloo@helmholtz-berlin.de

Anion exchange membranes (AEMs) are central to the performance of redox flow batteries (RFBs), where they must provide high ionic conductivity, low crossover of the redox-active species, and sufficient chemical and mechanical stability at a reasonable cost [1,2]. Commercial fluorinated membranes such as Fumasep satisfy several of these requirements but remain expensive and difficult to tailor. As perfluorinated materials, they also raise sustainability concerns, since they are environmentally persistent and increasingly regulated as forever chemicals [3]. Here, we report a poly(phenylene oxide) (PPO)-based AEM prepared by Friedel-Crafts acylation, followed by quaternization and crosslinking with poly(ethylene glycol) (PEG) to improve water management and dimensional stability. The PEG segments provide controlled hydrophilicity and a flexible crosslinked network, limiting water uptake and swelling while preserving efficient ion transport. The membrane structure was confirmed by FTIR and ¹H NMR, and its thermal properties were evaluated by DSC and TGA. Water uptake, swelling ratio, IEC, and ionic conductivity were also determined. The optimized membrane exhibits an IEC of 1.5 meq/g, a water uptake of 35%, a hydration number of 12.4, and a Cl⁻ conductivity of 4.8 mS/cm at 25 °C, exceeding the values obtained for the commercial Fumasep membrane. In a TMA-TEMPO/methyl viologen RFB, the membrane delivered a coulombic efficiency of 98.9%, a voltage efficiency of 86.2%, and an energy efficiency of 85.2% at 15 mA/cm², outperforming the Fumasep FA-3-50 reference under identical conditions with stable operation over 200 cycles. These results indicate that PEG crosslinking of quaternized PPO offers a cost-effective route to high-performance AEMs for RFB applications.

ABSTRACTS OF POSTER PRESENTATIONS

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ABSTRACTS OF POSTER PRESENTATIONS

P 81: Dry-processed activated carbon symmetric electrode performance of static zinc-bromine battery

Chan Sol Park¹, Tae Hun Kang², Ho Seok Park^{1,2}

¹School of Future Energy Engineering, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

²School of Chemical Engineering, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

pcs970701@skku.edu

Static Zinc-Bromine batteries (ZBBs) are attractive for low-cost and safe energy storage because they employ aqueous electrolytes and earth-abundant materials. However, conventional slurry-based electrode fabrication requires solvent handling and energy-intensive drying. In this study, thick activated carbon electrodes were fabricated through a solvent-free dry process using fibrillated polytetrafluoroethylene (PTFE) binder. The resulting electrodes exhibited a mechanically integrated carbon framework suitable for bromine redox reactions. A symmetric-cell configuration was employed to isolate the Br⁻/Br₂ redox chemistry from Zn plating/stripping and to directly evaluate the electrochemical behavior of the dry-processed electrodes. In addition, tetraethylammonium bromide (TEABr) was introduced into the ZnBr₂ electrolyte to regulate polybromide species and suppress their migration. The dry electrodes showed reversible bromine redox behavior and stable galvanostatic cycling over areal capacities of 2.0–5.0 mAh cm⁻² at 10 mA cm⁻², maintaining 83.2% capacity retention at 5.0 mAh cm⁻². At 2.5 mAh cm⁻², the TEABr-containing symmetric cell operated for 2,000 cycles with a coulombic efficiency of approximately 93%, whereas the cell without TEABr exhibited pronounced capacity fading. These results demonstrate that dry-processed activated carbon thick electrodes, combined with polybromide regulation by TEABr, provide a scalable and environmentally favorable electrode strategy for static ZBBs.

ABSTRACTS OF POSTER PRESENTATIONS

P 82: Novel fully recyclable polymeric cathode material for sustainable organic batteries

Laura Plein, Prof. K. Meerholz*

Institute of Light and Matter Chemistry, University of Cologne

laura.plein@uni-koeln.de

In recent years, organic battery materials have attracted great attention in energy storage. Since the sustainability of the inorganic materials commonly used in batteries today becomes more of an issue, finding alternatives becomes essential. Employing organic materials as electrode materials has turned out to show promising advantages such as mechanical flexibility, tuneable properties, sustainability and safer handling. However, obtaining organic materials requires several synthetic steps including sometimes environmentally harmful solvents or chemicals. Life cycle assessment has shown that the use of organic materials in batteries can have a larger environmental impact than commercially used inorganic materials.^[1] By making the organic material recyclable and therefore reusable, the environmental impact can be significantly reduced.

Here, we have synthesized recyclable polymers containing triphenylamine (TPA) as redox active unit. Application as cathode material in coin cells with Li metal as anode showed a high potential of over 3.9 V and a specific capacity of up to 55 mAh g⁻¹ at 1C. After cycling the batteries over 5000 times, the capacity decreased by 50%. Afterwards, the cell was disassembled, and the cathode was removed and recycled by depolymerizing the active material to recover the monomers. The monomers were extracted, purified and then polymerized again to undergo the next use cycle. Introducing the possibility to recycle the active material is a promising method to overcome the environmental burden of organic materials.

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ABSTRACTS OF POSTER PRESENTATIONS

P 83: Recyclable organic binders for cathode materials

Pourya Salehi, Heike Klesper, Klaus Meerholz

Institute for Light and Materials, Department of Chemistry and Biochemistry,
University of Cologne, Greinstr. 4-6, 50939 Cologne, Germany

psalehi2@uni-koeln.de

Lithium-ion batteries (LIBs) are a key technology for mobile and stationary energy storage, but they also pose challenges. LIBs with inorganic cathode materials rely on critical raw materials such as Co, Ni, and Mn, associated with social, environmental, and geopolitical issues and for which the EU faces high levels of strategic dependence. Organic cathode materials are generally even more expensive and less environmentally friendly than the currently established inorganic materials due to the many synthesis and purification steps involved in their production ^[1].

Binders are used in both inorganic and many low-molecular-weight organic cathode materials. Their purpose is to ensure the mechanical integrity of the cathode. This is necessary to achieve high cycle stability and good adhesion to the current collector. In inorganic LIB, polyvinylidene fluoride (PVDF) is often used as the binder, a perand polyfluoroalkyl substance (PFAS), which it is classified as a so-called “forever chemical” causing environmental and health problems. For both organic and inorganic cathode materials, the problems mentioned above would be mitigated by efficient recycling of the cathode materials and the use of PFAS-free binders.

In this work, we investigated a new class of halogen-free, i.e. PFAS-free binders for both organic and inorganic cathode materials. After use these materials can be easily decomposed into the original monomers by depolymerization. This allows for both the previously bound cathode materials and the binder itself to be easily and efficiently released, separated and reused. The simplified recovery process improves the end-of-life recycling of the cathode materials used and reduces the consumption of energy and raw materials. We will show the comparison of this new class of recyclable binders with conventional binders.

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ABSTRACTS OF POSTER PRESENTATIONS

P 84: Scalable hybrid electrode-based capacitive deionization modules for practical water softening

Sang Baek Kim^{1,†}, Gun Jang^{2,†}, Wonji Jung^{3,†}, Hye Rin Park², Youngkyu Cho³, Sung Pil Hong³, Jee Yeon Kim³, Changhoon Oh³, Ho Seok Park^{1,2,4,5,6}

¹Department of Future Energy Engineering, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

²Department of Chemical Engineering, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

³Samsung Research, Samsung Electronics Co., Ltd., Seoul, Republic of Korea

⁴SKKU Institute of Energy Science and Technology (SIEST)

⁵SKKU Advanced Institute of Nano Technology (SAINT)

⁶Samsung Advanced Institute for Health Sciences and Technology (SAIHST), Sungkyunkwan University (SKKU), Suwon, Republic of Korea

adfkg12@o365.skku.edu

Battery-type faradaic electrodes are developed for energy storage, yet the same redox chemistry can be redirected to pull ions out of water. Capacitive deionization (CDI) built on activated carbon (AC) is limited by the low areal ion capacity of purely capacitive storage, which becomes the bottleneck once the technology is scaled toward household water softening. Here we report a vanadium-oxide hybrid (VH) electrode in which V₂O₅ and AC (7:3 by weight) are roll-to-roll coated onto a graphite current collector, coupling faradaic V⁵⁺/V⁴⁺ ion storage with double-layer adsorption: the faradaic contribution raises capacity and rate, while the carbon fraction preserves the cyclability of carbon-based CDI.

On the intended hard-water feed (250 mg L⁻¹ total dissolved salt; CaCl₂/MgCl₂ at a Ca²⁺:Mg²⁺ molar ratio of 5:1) at ±1.2 V, and quantified with community-standard metrics ^[1], the VH cell delivers a salt adsorption capacity of 2.09 mg g⁻¹ and an average salt adsorption rate of 0.582 mg g⁻¹ min⁻¹, against 1.68 mg g⁻¹ and 0.394 mg g⁻¹ min⁻¹ for a symmetric AC/AC cell measured under identical conditions, with an areal capacitance of 2.00 F cm⁻² versus 1.66 F cm⁻². Capacity, rate and 300-cycle stability (93.2% retention) are reported on the same feed, a combination seldom reported together for divalent-targeted CDI electrodes ^[2], and post-cycle XRD preserves every α-V₂O₅ reflection ($|\Delta 2\theta| \leq 0.031^\circ$).

COMSOL simulations coupling laminar flow, Nernst–Planck ion transport and Donnan equilibrium at the ion-exchange membranes identified a rectangular short-electrode geometry, which was carried into a bipolar multistack module of 105 stacks (125.5 × 160 mm² electrodes; 42,168 cm² total active area) operated at 1.5 V per cell. The module removes 89.9% of the influent ions at 0.5 L

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min^{-1} and 83.7% at 2.5 L min^{-1} , the flow range of a household dishwasher, and sustains $\approx 83\%$ removal on real tap water. A battery-type electrode carried through a scalable coating process therefore transfers its faradaic advantage intact from the single cell to a liter-per-minute water-treatment module^[3].

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ABSTRACTS OF POSTER PRESENTATIONS

P 85: GEL-based electrodes for electro-swing adsorption of dilute CO₂ (<1%)

Pavan Kumar Vudisi, Sina Azad, Michael Bauer, Jakob Heier, Roland Hany, Frank Nüesch

Laboratory for Functional Polymers, Swiss Federal Laboratories for Materials Science and Technology (Empa), Überlandstrasse 129, 8600 Dübendorf, Switzerland

pavan.vudisi@empa.ch

Global temperature rise necessitates reducing greenhouse gas emissions, particularly CO₂. Alongside renewable energy deployment, carbon capture from dilute streams and point sources is critical for achieving net-zero targets. Conventional sorbent-based technologies often require substantial energy for regeneration, whereas electrochemical CO₂ capture offers potentially lower energy demand, modular operation, and compatibility with renewable electricity. In redox-active molecule-mediated systems, such as anthraquinone (AQ)-based organic flow batteries, CO₂ capture occurs through electrochemically generated nucleophiles. However, low solubility of redox-active molecules, restricted CO₂ transport, and limited active-site accessibility can constrain capture performance. Here, graphene GEL electrodes incorporating functionalized anthraquinone (FAQ) are developed for electro-swing CO₂ capture in an organic flow battery architecture. AQ was functionalized with imidazolium side chains to enhance solubility in ionic liquid electrolytes. FAQ retains redox behavior comparable to AQ, while the GEL architecture provides a continuous ionic environment, improved interfacial accessibility, and facilitated CO₂ transport. Capture/release experiments achieve ~1 mol CO₂ per mol FAQ at 0.36% CO₂ and ~0.5 mol CO₂ per mol FAQ at 0.06% CO₂. These results demonstrate that combining molecular functionalization with flow-battery electrode architecture is a promising strategy for electrochemical CO₂ capture from dilute streams.

NOTES

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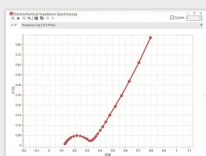
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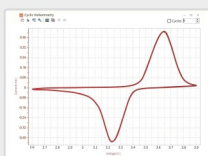
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CONTACT

Friedrich Schiller University Jena
Center for Energy and Environmental Chemistry Jena (CEEC Jena)
Prof. Dr. Ulrich S. Schubert
Ms. Sylvia Braunsdorf
Philosophenweg 7a
07743 Jena
Germany

Phone: +49 3641 9-48236
Fax: +49 3641 9-48202
Email: obd2026@uni-jena.de

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