Organic Battery Days 2023

Donostia-San Sebastian
June 7th-8th 2023

EUSKO JAURLARITZA
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DEPARTAMENTO DE EDUCACIÓN

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Welcome/Bienvenidos/Ongi Etorri

Welcome to the 6th Organic Battery Days at the University of the Basque Country on June 7–8, 2023. This continues a series of Organic Battery Days events that started in Uppsala, Sweden in 2017, and it has been subsequently held in Tianjin (China), Jena (Germany), Waseda (Japan) and Houston (USA). This year the Organic Battery Days will be held in Donostia-San Sebastian, Spain.

Organic Battery Days is a yearly reference event for organic battery experts. In this meeting we will discuss the most recent developments in the field of organic batteries, such as the design and synthesis of organic electroactive materials, study of these materials in various electrochemical systems (e.g., rechargeable batteries, flow cells), and electrolytes for organic electrodes. This meeting will be held in person.

OBD2023 will count with the participation of 100 researchers coming from all around the world. We would like to thank all our generous sponsors and the volunteers that will help us to make it a successful conference.

We look forward to an inspiring meeting that will generate innovative ideas in this exciting field of research and development.

Sincerely,

Nerea Casado & David Mecerreyes
OBD2023 Chairs

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Congress Venue

Miramar Palace

Pº de Miraconcha nº 48. Donostia / San Sebastián
Gipuzkoa

Congress Dinner Venue

Gastronomiazko Euskal Anaiartea -Cofradía Vasca de Gastronomía

Elvira Zipitria s/n, 20003 Donostia - San Sebastián, Gipuzkoa

https://www.gastronomica.com/la-gastronomica/

Pre-Conference Workshop

POLYSTORAGE

MSCA – European Training Network – POLYSTORAGE

6th POLYSTORAGE Workshop
"From R&D activities in next-generation batteries to industrial exploitation"

6th June

14:00- 19:00
Venue: : Joxe Mari Korta Center, UPV/EHU, Donostia-San Sebastian
Organizers :
Rebeca Marcilla (IMDEA Energy, Spain)
David Mecerreyes (POLYMAT, Spain)
INFO & REGISTRATION

Satellite event to the Organic Battery Days 2023

Description: This half-day workshop is addressed to PhD students and young researchers within the POLYSTORAGE ETN as well as OBD 2023 participants, but also open for everyone interested upon registration. It will be dedicated to shed some light into skills for industrial researchers including IPR issues, commercial exploitation of results, entrepreneurship and creation of start ups, leadership skills in industry, industrial research management, transfer of technology, etc. The WS includes an excellent line-up of international speakers with broad experience in those topics.

		Name	Position	Institution/Company	TITLE
	14.00-14.45	Prof. Adelio Mendes / Dr. Paula Dias	Senior Researcher and Coordinator of the Research group: Processes, Products and Energy / Junior researcher	Faculty of Engineering at the University of Porto (Portugal)	From the fundamentals to the start-ups: a refreshed way to design the research
	14.45-15.30	Dr. Juan Pablo Esquivel	Co-founder and Scientific Advisor, Fuelium. Ikerbasque Research Associate, BCMaterials	Fuelium/BCMaterials (Spain)	Fuelium. The story of spinning off a paper battery company from the lab and some of the lessons learned so far.
	15.30-16.15	Enrique Serrano	Co-Founder	B5Tech (Spain)	First Organic Hybrid Supercap
	16.15-16.45			*Coffee Break*	
	16.45-17.30	Dr. Tobias Janoschka	Chief Technical Officer / Founder	Jenabatteries GmbH (Germany)	Turning Scientific Innovation into Business
	17.30-18.15	Aldo D'Ambrosio	Business Development - Battery Cells Solution Owner Strategic Marketing and Solutions Management	COMAU S.p.A (Italy)	Comau path - Industrializing the Innovation
	18.15-19.00	Dr. Tajna Benedict	Head of Legal Services & IP	InnovationLab (Germany)	From scientific results to commercialization

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 860403.

Conference Program

Wednesday, June 7th 2023	
8:15 - 8:45	***Registration***
8:45 – 9:00	***Opening ceremony***
9:00 - 9:45	**PL1: Kenichi OYAIZU** *Waseda University, Japan* Polymers for Energy Storage: Organic Batteries and Hydrogen Carriers
9:45-10:10	**I1: Birgit ESSER** *Ulm University, Germany* Advancing the properties of phenothiazine-based redox polymers as positive electrode materials in batteries
10:10-10:35	**I2: Jan BITENC** *National Institute of Chemistry, Ljubljana, Slovenia* Application of organic cathodes to multivalent (Mg, Ca, Al) metal anode-organic batteries
10:35-11:00	**I3: Nicolas GOUJON** *POLYMAT, University of the Basque Country UPV/EHU* Dual redox active polymers towards high energy density cathode materials
11:00-11:30	***Coffee Break***
11:30-11:55	**I4: Nagaraj PATIL** *IMDEA Energy, Spain* Practical Li-ion Batteries with High-Performance Polyimide Electrodes
11:55-12:20	**I5: Matthieu BECUWE** *UPJV-LRCS, France* Anion-insertion molecular materials based on heterocyclic aromatics, toward high-voltage and energy density dual-ion battery?
12:20-12:45	**O1: Manuel SOUTO** *University of Aveiro- CICECO, Portugal* Organic batteries based on redox-active Covalent Organic Frameworks: challenges and opportunities
12:45-13:10	**O2: Nara KIM** *Linköping University, Sweden* Intrinsically Stretchable Symmetric Organic Battery Based on Plant-Derived Redox Molecules
13:10-13:35	**O3: Thibaut GUTEL** *CEA, France* Towards Full Li-ion Prototype Based On Organic Electrode Materials
13:35-14:45	***Lunch***

14:45-15:30	**PL2: Jodie LUTKENHAUS** *Texas A&M University, USA* Toward Recyclable or Degradable Organic Polymer Batteries
15:30-15:55	**I6: Ji Eon KWON** *Korea Institute of Science and Technology (KIST), Korea* Nature-derived Organic Molecules for Low-cost and Sustainable Electrode Materials
15:55-16:20	**O4: Klemen PIRNAT** *National Institute of Chemistry, Slovenia* Polyphenol Cathode Material
16:20-16:55	***Coffee Break***
17:00-18:10	**Flash Presentations**
18:10-19:30	**Poster Session**

Thursday, June 8th 2023

9:00 – 9:45	**PL3: Yan YAO** *University of Houston, USA* Organic Electrode Materials for Magnesium and Solid-state Batteries
9:45-10:10	**I7: Zhongfan JIA** *Flinders University, Australia* Exploring Two-electron Storage in Radical Polymer Batteries
10:10-10:35	**I8: Philippe POIZOT** *Nantes Université, CNRS, France* Investigations of the electrochemical delithiation/lithiation process in magnesium (2,5-dilithium-oxy)-terephthalate
10:35-11:00	**O5: Stéven RENAULT** *Nantes Unversity-IMN/CNRS, France* Towards Extreme Capacities for Organic Electrode Materials: Stabilizing Superlithiation Phenomenon
11:00-11:30	***Coffee Break***
11:30-11:55	**I9: Eduardo SANCHEZ** *CIC energiGUNE, Spain* AORFB: design, synthesis and integration of organic materials
11:55-12:20	**I10: Rebeca MARCILLA** *IMDEA Energy, Spain* Unprecedent Capacity of non-functionalized TEMPO Catholyte and their application in Aqueous Redox Flow Batteries
12:20-12:45	**I11: Vijay MURUGESAN** *Pacific Northwest National Laboratory, USA*

	Data Science based Electrolyte Design for Organic Redox Flow Batteries
12:45-13:10	**O6: Guiomar HERNANDEZ** *Uppsala University, Sweden* Self-healing binders with boron-based linkers
13:10-13:35	**O7: Joel GAUBICHER** *CNRS, Nantes, France* Organic electroactive based aqueous ion-batteries for energy storage and water desalination
13:35-15:00	***Lunch***
15:00-15:45	**PL4: Ulrich S. SCHUBERT** *Friedrich Schiller University Jena, Germany* Polymer-based redox flow batteries and solid-state polymer batteries
15:45-16:10	**I12: Jean Francois GOHY** *Université Catholique de Louvain, Belgium* Introducing smart functionalities in solid polymer electrolytes
16:10-16:35	**O8: Edgar VENTOSA** *University of Burgos, Spain* Addressing Practical Use of Viologen-Derivatives in Redox Flow Batteries through Molecular Engineering
16:35-17:00	**I13: Daniel BRANDELL** *Uppsala University, Sweden* Discovering redox-stable organic battery electrodes using AI
17:00-17:25	**O9: Masaru YAO** *National Institute of Advanced Industrial Science and Technology (AIST), Japan* Improvement in current collecting property of organic positive electrode and its electronic conduction mechanism
17:25-17:40	***Closing Remarks***
20:30	***Conference Dinner*** ***Location: Sociedad Gastronomica*** https://www.gastronomica.com/la-gastronomica/

List of Flash Presentations and Poster

Flash	Person and Title
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Poster 2	**Tijs Lap** Bio-based Polyhydroxyanthraquinone Redox Polymers as High-Voltage Organic Cathode materials for Lithium-Ion Batteries
Poster 3	**Alessandro Innocenti** A holistic approach to the design of practical polymer organic batteries
Poster 4	**Isaac Alvarez Moises** Liquid crystals as additives in solid polymer electrolytes for lithium metal batteries
Poster 5	**Pierre Stigliano** PDADMATFSI-Poly(Vinyl Benzoate) Triblock Copolymers for Sodium Metal Battery Applications
Poster 6	**Olivera Lužanin** Multivalent Ion Transport in Organic Electrodes: A Microscopic Study
Poster 7	**Ousmane Camara** (Metal-)Organic Battery based on PANI/Polycatechol Hybrid
Poster 8	**Yinghui ZHANG** Design of novel types of hybrid polymer/inorganic solid electrolytes with enhanced ionic conductivities
Poster 9	**Shanshan Yan** Polyrotaxane-based networks as electrolytes and catholytes for all solid-state lithium batteries
Poster 10	**Tjaša Pavčnik** A novel fluorinated alkoxyaluminate-based electrolyte for Ca batteries
Poster 11	**Ying Zhang** Development of Advanced All-Solid-State Polymer Electrolytes Using Innovative, Rapid, and Solvent-Free Procedures
Poster 12	**Svit Menart** Novel organic cathode materials based on pyrazine and quinone motifs for rechargeable lithium-ion and zinc-ion batteries
Poster 13	**Robert Markowski** High performance coordination polymers for post-Li battery technologies
Poster 14	**Laura Pastor** Novel Organic Redox-Active Compounds for Next Generation Redox Flow Batteries
Poster 15	**Carlos Villacis** PDDAFSI-PYR13FSI-LiFSI-LLZO hybrid electrolytes for high- voltage solid state lithium metal batteries
Poster 16	**Marina Navarro Segarra** An ecodesigned cardboard primary battery for smart packaging applications
Poster 17	**Ashish Raj** Investigating Bio-derived Polyhydroxy urethanes network bearing carbonates as solid polymer electrolyte
Poster 18	**Kai Shi** Self-Organized High-Energy Organic Electrodes

List of Poster

Poster #	Person and Title
Poster 19	**Martin, Karlsmo** Low-cost and sustainable aqueous lithium-ion batteries by all- organic PTCDI anodes
Poster 20	**Raquel Dantas** Lithium-ion battery electrode materials based on redox-active Covalent Organic Frameworks
Poster 21	**Philipp Penert** Cationic Viologen Polymers in Anion Rocking-Chair Batteries and Full-Organic Cells
Poster 22	**Xiaotong Zhang** Discovery of degradation mechanisms of organic redox flow battery(RFB) electrolytes
Poster 23	**Alba Fombona Pascual** Organic faradaic deionization cell based on polyimide symmetric electrodes
Poster 24	**Géraldine Chanteux** One-step non-sacrificial electrodeposition of an electrically conducting MOF on various functional substrates and microdevice integration
Poster 25	**Karol Jagodzinski** Novel binders enabling Si-rich anodes for the next generation Li-ion batteries
Poster 26	**Robin Wessling** Unlocking reversible twofold oxidation in N-styrylphenothiazine-based polymers
Poster 27	**Hyojin Kye** Indolocarbazole-Based Small-Molecules as p-Type Cathode Materials with Double Redox for Lithium-Organic Batteries
Poster 28	**Gauthier Studer** Electrochemical investigation of a phenothiazine polymer as positive electrode material for aluminium batteries
Poster 29	**Tom Goossens** Lithium-Phenolate (Metal-)Organic Cathodes
Poster 30	**Vasudeva Rao Bakuru** Visible-Light Augmented Lithium Storage Capacity in a Ruthenium (II) Photosensitizer Conjugated with a Dione Catechol Redox Couple
Poster 31	**Shirin Shakouri** Molecular Engineering of Metalloporphyrins for High- Performance Energy Storage: Central Metal Matters
Poster 32	**Sibylle Riedel** Quinone-based Cathodes in Magnesium and Calcium based Batteries using non-corrosive [B(hfip)4]-Electrolytes
Poster 33	**Somayeh Ahadi** Organic redox polymers for multivalent ion batteries
Poster 34	**Luisa Rzesny** Enhancing the Charge Storage Capabilities in Carboxylate-based Materials by Thiadiazole Fusion
Poster 35	**Manik Eknath Bhosale** Triazatruxene-based Covalent Organic Framework as Cathode Material for Organic Lithium Batteries
Poster 36	**Florin Adler** Multivalent Metal Batteries with Organic Electrode Materials
Poster 37	**Öykü Simsek** Novel gel polymer electrolytes for LI/PTMA cells

Poster 38	**Carles Tortosa Valdés** Biodegradable and compostable batteries for precision agriculture and decentralized energy systems
Poster 39	**Philip Zimmer** Distribution of relaxation times analysis of a hydrogel electrolyte for organic batteries
Poster 40	**Alessandro Michieletto** Water soluble polymers for redox-flow batteries
Poster 41	**Chinmaya, Mirle** Pentacene-5,7,12,14-tetraone based polymers as cathodes for sodium batteries
Poster 42	**Riccardo Alessandri** Morphology-Electronic Property Relationships in Radical-Containing Polymers for All-Organic Batteries
Poster 43	**Md. Adil** Pillar[5]quinone as a high-capacity organic cathode with a highly concentrated electrolyte for rechargeable Na-ion batteries
Poster 44	**Cleber Marchiori** Modelling the Li-ion insertion in organic electrode materials: energy minimum vs. metastable phases
Poster 45	**Aaron Peng** FAIR data-empowered active learning for the accelerated discovery of redox-active polymers for metal-free batteries
Poster 46	**Mathieu Branca** Disentangling the charge storage mechanism of quinone-based organic electrode materials in aqueous electrolytes
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Poster 48	**Sathiya Priya Panjalingam** A step towards Sustainability – Aqueous Processing of Organic Redox Polymers for Next-Generation Organic Batteries
Poster 49	**Rambabu Darsi** Revealing the Reversible Solid-State Electrochemistry of Lithium-Containing Conjugated Oximates: Towards a New Functionality for Organic Batteries
Poster 50	**Gangbing Song** Monitoring the State of Charge of Organic Batteries Using Ultrasonics
Poster 51	**Kenza Elbouazzaoui** Understanding the Ionic Conduction in Solid Polycarbonate-Garnet Composite Electrolytes

Oral Presentations

ABSTRACT PROPOSAL

POLYMERS FOR ENERGY STORAGE: ORGANIC BATTERIES AND HYDROGEN CARRIERS

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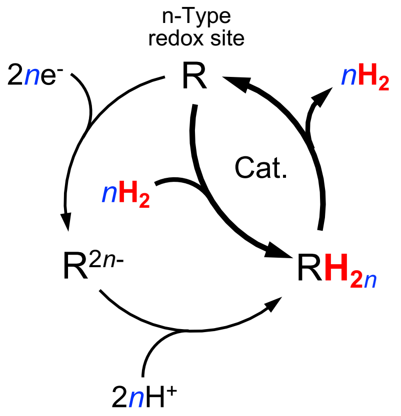
Keywords: *organic electrode, polymer, charge transfer, self-exchange reaction*

ABSTRACT

Redox-active polymers with charging/discharging reversibility and rapid electrode reaction rates are employed to develop organic electrode-active materials in organic batteries. The reversible charge storage with the aliphatic redox polymers is accomplished by the electron self-exchange reactions of the adjacent redox-active sites populated in the polymer layer, giving rise to the charge propagation throughout the layer to allow full charging and discharging. The organic batteries are characterized by high power-rate, flexible/bendable, and environmentally benign properties. Recently, many types of organic batteries are being developed, such as organic redox flow batteries and organic/inorganic hybrid batteries.

Negative charging of the electroneutral redox polymers results in a significant increase in basicity to allow protonation of the redox-active (Scheme). Since most of the hydrogenated products are no longer redox-active, aprotic battery electrolytes are employed to avoid the undesired hydrogenation in organic batteries. On the other hand, organic compounds that undergo reversible hydrogenation, such as toluene to yield methylcyclohexane, have been studied as hydrogen storage materials. However, the hydrogenation with hydrogen gas usually proceeds via a highly energy consuming process. We have found that various types of ketone-containing polymers stored hydrogen via the electrolytic process in the presence of water at room temperature. The resulting alcohol polymer evolved hydrogen (H_2) gas by warming under mild conditions with an iridium catalyst, which corresponded to the acceptorless oxidation of the hydrogenated product.

The hydrogenation/dehydrogenation cycle was accomplished throughout the polymer layer, meaning that all of the ketone groups in the polymer were equilibrated with the hydrogen gas according to $>C=O + H_2 \rightleftarrows >CH\text{-}OH$. The reversible hydrogenation/dehydrogenation was extended to many types of organic groups in the polymer, such as fluorenone, quinoxaline, quinaldine, pyrazine, pyridinopyrazine, and cyclic esters, providing the hydrogen carrier polymers as a new class of energy-related functional polymers.



Scheme Electrohydrogenation of n-type redox site R through electro-reduction and protonation, and reversible catalytic hydrogenation of R according to $R + nH_2 \rightleftarrows RH_{2n}$.

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ABSTRACT PROPOSAL

Advancing the properties of phenothiazine-based redox polymers as positive electrode materials in batteries

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Keywords: *phenothiazine, positive electrode materials, two-electron redox, aluminium batteries, all-organic batteries*

ABSTRACT

Phenothiazine is an attractive redox-active group for p-type positive electrode materials in batteries.[1] It is characterized by a two-electron redox reaction with fast kinetics, the reversibility of which depends on the substitution pattern, and multiple possibilities for functionalization. These allow the incorporation of phenothiazine into redox-active polymers, either into aliphatic polymers as a side group or as part of the main chain in conjugated polymers, affecting both the electronic conductivity and the morphology of the polymers.[2] The choice between linear and crosslinked polymers also allows their solubility properties in battery electrolytes to be adjusted.[3,4] By attaching substituents to the phenothiazine core that change its electronic character, both the redox potential and the stability of the oxidized states of phenothiazine can be affected.[5–7]
In this talk, I will present design principles for phenothiazine-based redox polymers to modify their redox and other properties for use as positive electrode materials in batteries. Examples include the development of a reversible two-electron redox process of each phenothiazine unit, the use of phenothiazine-based polymers in aluminium and all-organic batteries, and the use of phenothiazine redox polymers in photo-chargeable batteries enabled by their fast-charge capability.

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ABSTRACT PROPOSAL

Application of organic cathodes to multivalent (Mg, Ca, Al) metal anode-organic batteries

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Keywords: *multivalent batteries, organic cathodes, electrochemical mechanism*

Multivalent (Mg, Ca, Al) metal anodes offer highly promising gravimetric and volumetric capacities and are a promising option for future high-energy density batteries. However, their practical application is severely limited due to difficult insertion, slow-solid state diffusion and presence of side reactions. Organic cathodes with their relatively soft and adaptable structures offer an alternative to bypass the limitations of inorganic hosts.

In our work, we have combined conjugated carbonyl compounds in combination with different multivalent non-nucleophilic electrolytes. As a model compounds, we have utilized polymers from anthraquinone class, which with their moderate working potential fit well into the operating window of most multivalent electrolytes. Anthraquinone based compound display good electrochemical reversibility with moderate capacity utilization. Long-term cycling stability can in combination with insoluble organic polymers and suitable non-nucleophilic electrolytes reach several hundreds of cycles. Electrochemical mechanism was investigated with the plethora of characterization techniques like *operando* ATR-IR, *ex situ* SEM-EDS, XPS and solid-state NMR. Detailed characterization has identified presence of multivalent cation-anion pairs, which identifies important challenge for future research.

ABSTRACT

Dual redox active polymers towards high energy density cathode materials

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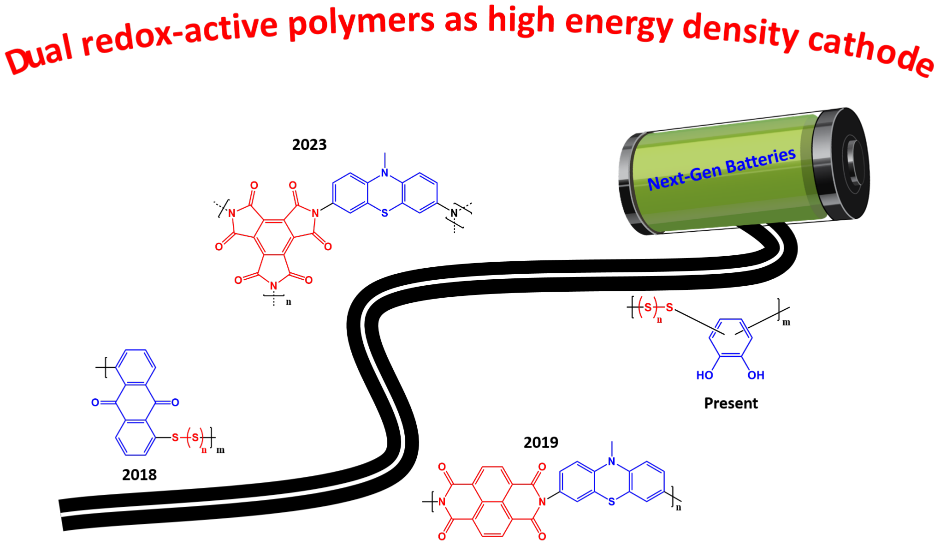
Keywords: *dual redox-active, redox polymer, organic cathode, lithium metal batteries*

Redox polymer is considered as a promising cathode material for the next generation of batteries due to their inherent attributes such as sustainability, processability, low solubility compared to small molecule analogues and high rate capability However, the development of high energy density cathode materials based on redox polymer, by either increasing their theoretical capacity or redox potential, still remains a challenging task. Our research group was one of the pioneer to explore the concept of dual redox-active polymer for the development of high energy density cathode material.[1–3] Indeed, some of the most studied redox polymers, such as poly(anthraquinoyl sulphide) and polyimide, employed an non redox-active linker, decreasing the theoretical capacity of the polymer. Herein, we present some of our recent works on the development of dual redox-active polymers, based on either porous polyimide or bio-inspired poly (catechol sulphide) chemistry, and their application as cathode materials for high energy density lithium metal batteries.



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ABSTRACT PROPOSAL

Practical Li-ion Batteries with High-Performance Polyimide Electrodes

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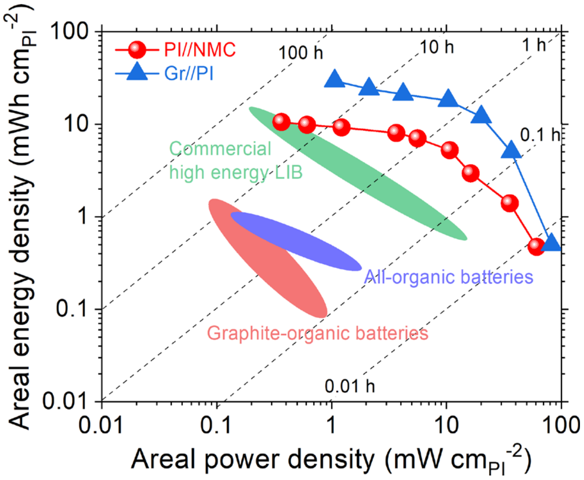
Keywords: *Organic electrode materials, redox-active polymers, Li-organic battery, high areal capacity*

ABSTRACT

Redox-active polymers (RAPs) are anticipated to be promising organic electrode materials for the development of more sustainable, economical, and safer batteries. However, their high electrochemical performance is inherently associated with the use of low mass-loading electrodes (typically below 2 mg cm^{-2}) with high carbon-additives content (20–80 wt%), which collectively hinders their practicability in real batteries.[1] In this talk, I will present an interesting approach for developing high-performance and practical 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTCDA)-derived polyimide (PI) electrodes that are processed into self-supported, current collector-free buckypaper electrodes. This effective electrode fabrication method enables high-mass-loading composite electrodes (up to 55 mg cm^{-2}) with low carbon-additives content (30 wt %), which attained high gravimetric (155 mAh g^{-1}), areal (10 mAh cm^{-2}) and volumetric (202 mAh cm^{-3}) capacities with good rate capability (1.6 mAh cm^{-2} at 5C) in Li-ion half-cells. These are most probably the highest values reported for an organic electrode in Li-ion batteries, constituting a great leap forward in the development of practical organic batteries. As a proof of concept, semi-organic full cells were assembled in Graphite||PI, LTO||PI, PI||LFP, and PI||NMC configurations in both coin-type and pouch-type cell prototypes to assess the practicality of these high-mass-loading PI electrodes. The electrochemical performance metrics in terms of capacity, energy and power density (gravimetric, volumetric and areal) of these full cells were assessed, along with preliminary cost prediction of practical Li-ion batteries for e-mobility application.[2] Both the performance metrics and cost factors for the presented redox polymers were favorable that could have great prospects for future practical (semi)organic batteries.



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ABSTRACT PROPOSAL

Anion-insertion molecular materials based on heterocyclic aromatics, toward high-voltage and energy density dual-ion battery?

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Keywords: *molecular materials, anion insertion, dual-ion battery, heterocyclic aromatics*

ABSTRACT

For more than fifteen years, research on a new generation of batteries incorporating organic materials has been strongly developed, allowing the construction of less expensive and more environmentally friendly batteries. In addition to the abundance of elements used to manufacture these materials (C, N, H, O, S, etc.) and the ease of recycling, a definite advantage is the possibility of working with anions as a mobile species. Two types of batteries are thus possible: the anionic battery (rocking-chair of the anion instead of lithium or sodium) and the dual-ion battery (using the salt of the electrolyte as a charge reservoir). The latter combines two types of materials, namely an *n*-type at the negative (cation insertion) and a *p*-type at the positive (anion insertion). To date, the positive materials are attracting the most attention since for the negative electrode, graphite or lithium carboxylates can be used.

In recent years, various studies have been carried out on positive electrode materials with the aim of improving the performance of these systems. [1-2] In this context, our group is interested in the control of the electrochemical properties of electrode materials based on heterocyclic aromatic compounds. Our attention has been focused on carbazole,[3] phenothiazine[4] and thianthrene type motifs for which different strategies have been implemented to modulate the redox potential, the reversibility of the electrochemical reaction or the solubility of the molecular material, the final objective being to maximise the storage performance in order to build high energy density assemblies.

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Organic batteries based on redox-active Covalent Organic Frameworks: challenges and opportunities

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Keywords: *Organic electrode, redox-active Covalent Organic Frameworks, electroactive organic materials*

ABSTRACT

A major breakthrough in chemistry and materials science has been the development of Lithium-Ion Batteries (LIBs), which show great potential for storing energy from renewable sources and as the power source for electric cars.[1] However, commercially available LIBs are based on transition metal oxide cathodes, presenting limited energy density and raising relevant environmental concerns. Organic materials have received much attention as alternative electrodes because of their high theoretical capacity, resources availability and sustainability.[2,3] In particular, Covalent Organic Frameworks (COFs), crystalline porous polymers based on organic building blocks linked by strong covalent bonds, have emerged in the past few years as promising organic electrode materials due to their high stability, high ionic conductivity and outstanding chemical and structural versatility.[4] In this presentation, I will show some different examples of redox-active COFs used as cathode materials for coin-cell type lithium batteries highlighting some of its advantages and challenges in comparison with other organic electrodes. I will also focus on the COFs processing optimization to improve the batteries performance. Finally, I will highlight some strategies to improve the charge transport in COFs, one of the main bottlenecks of these organic electrode materials.[5]

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ABSTRACT PROPOSAL

Intrinsically Stretchable Symmetric Organic Battery Based on Plant-Derived Redox Molecules

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Keywords: *Organic Battery, Stretchable Electronics, Redox Molecules, Sustainable Electronics, Multi-functional Composites*

ABSTRACT (200 words max.)

Abstract text

Intrinsically stretchable energy storage devices are essential for the powering of imperceptible wearable electronics. Organic batteries based on plant-derived redox-active molecules can offer critical advantages from a safety, sustainability, and economic perspective, but such batteries are not yet available in soft and stretchable form factors. Here we report an intrinsically stretchable organic battery made of elastomeric composite electrodes formulated with alizarin, a natural dye derived from the plant *Rubia tinctorum*, whose two quinone motifs enable its uses in both positive and negative electrodes. The achieved self-organized hierarchical morphology of the quaternary biocomposite electrodes leads to excellent electron-ion conduction/coupling and superior stretchability (>300%). In a full-cell configuration, its energy density of 3.8 mWh cm^{-3} was preserved upon 100% tensile strain and 1000 stretching cycles at 50% strain, and assembled modules on stretchy textiles and rubber gloves can power integrated LEDs during various deformations. This work paves the way for low-cost, eco-friendly, and deformable batteries for next generation wearable electronics.

ABSTRACT PROPOSAL

Towards Full Li-ion Prototype Based On Organic Electrode Materials

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Keywords: *organic electrode material, Li-ion battery*

ABSTRACT

Nowdays electrode materials of Li-on batteries are mainly constituted by inorganic compounds based on transition metals (Co, Ni). Although their electrochemical performances are satisfying, these materials present several important drawbacks. Indeed they are expensive and present high environmental footprints.

N-type organic electroactive compounds offer a cost-effective and environmental friendly alternatives for electrochemical storage. Interestingly 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 the lack of lithium source.

In order to demonstrate the interest of organic battery technology at cell level, a lithiated air-stable compound, magnesium (2,5-dilithium-oxy)-terephthalate [$Mg(Li_2)$-p-DHT], has been produced at pilot scale in collaboration with IMN. Our optimizations lead to electrodes with high loading ($1mAh.cm^{-2}$) and low carbon content (<15%wt) and double-sided electrodes have been coated on CEA pre-industrial equipement. Finally full Li-ion prototypes (multi-layer prismatic cell of 160mAh) have been assembled and show 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.

ABSTRACT PROPOSAL

Toward Recyclable or Degradable Organic Polymer Batteries

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Keywords: *redox-active polymers, recycling, degradation*

ABSTRACT

Cobalt, nickel, and lithium are essential ingredients in today's lithium-ion batteries (LIBs), but their continued use presents economic, ethical, and environmental challenges. Society must now begin to consider the implications of a LIB's full life cycle, including the carbon footprint, the economic and environmental costs, and material access. These challenges motivate the case for degradable or recyclable batteries sourced from earth-abundant materials whose life cycle bears minimal impact on the environment. This presentation considers organic polymer-based batteries, which have the potential to address many of these issues. These electrodes consist of redox-active polymers that are compatible with aqueous or nonaqueous electrolyte. We demonstrate polypeptide radical batteries that degrade on command into amino acids and by-products as a first step toward circular organic batteries. Further, we show the recycling of redox-active polymer electrodes, and we discuss the new resulting challenges. To understand the mechanism of the redox-active polymer's reaction, we apply electrochemical quartz crystal with dissipation monitoring (EQCM-D) to analyze the real-time mass changes in the polymer. Therefore, the number of ions and solvent molecules transporting into and out of the electrode during cyclic voltammetry, galvanostatic cycling, and even electrochemical impedance spectroscopy is quantified.

ABSTRACT PROPOSAL

Nature-derived Organic Molecules for Low-cost and Sustainable Electrode Materials

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Keywords: *organic electrode materials, organic batteries, natural dyes, vitamins*

ABSTRACT

Redox-active organic materials (ROMs) are recently drawing much attention as promising alternatives to conventional electrode materials for rechargeable batteries owing to their natural abundance, low cost, easy chemical tunability, and large specific capacity. However, organic electrode materials are still plagued by slow rate performance, poor capacity utilization, and fast capacity fading, mainly due to their electrically insulating nature and high solubility. Various strategies have been proposed to address these issues, such as compositing with nanocarbons, polymerization, and substituting with multiple functional groups. Nevertheless, these approaches require complex synthesis, composite fabrication, or polymerization steps, naturally increasing preparation costs and environmental concerns.

In this talk, we introduce a series of natural organic dyes with simple molecular structures for low-cost electrode materials. These materials exhibit low solubility in organic electrolytes and form unique nanostructures in the electrode films due to strong intra-/inter-molecular secondary interactions, resulting in high cycle stability and superior rate performance. Additionally, we compare the electrochemical performance of water- and fat-soluble vitamins as electrode materials for aqueous batteries. Finally, we evaluate the bio-compatibility of the vitamin-derived electrodes. These results suggest a promising direction for developing sustainable and bio-compatible electrode materials with low cost for next-generation rechargeable batteries.

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4.

ABSTRACT PROPOSAL

POLYPHENOL CATHODE MATERIAL

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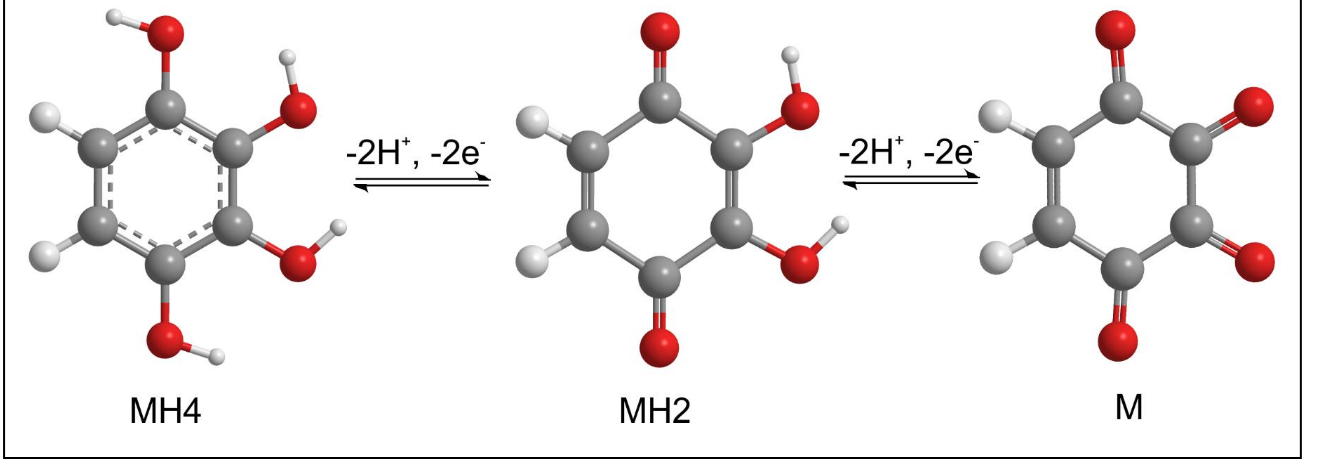
Keywords: *Polyphenols, organic cathodes, proton battery*

ABSTRACT

Organic batteries are a new battery technology that holds great potential to revolutionize energy storage. They are more sustainable than traditional Li-ion batteries. Redox-active materials offer higher specific capacities than their inorganic counterparts and they can be used in different electrolytes in the combination with different metals.

This study focuses on a range of hydroxybenzenes, from mono- to hexa-hydroxy, and identifies 1,2,3,4-tetrahydroxybenzene derivative (MH4) as the best candidate in terms of specific capacity and cycle stability. We were able to chemically synthesize half oxidized (MH2) and fully oxidized ($M \times 2H_2O$) derivatives of MH4. We show by using cyclovoltammetry that reversible electrochemical conversion is possible between three derivates. The highest electrochemical activity has been obtained in an aqueous solution of 0.1M $HClO_4$.

To enable stable cycling, we further developed polymer nanoparticles based on poly(2,3,4,5-tetrahydroxystyrene) with a high theoretical capacity of 631 mAh/g. When this cathode material was tested with organic electrolyte and Li metal anode, it showed no redox peaks and a very low capacity of 111 mAh/g. It seems that 1,2,3,4-tetrahydroxybenzene derivatives have similar properties as catechols and work much better in acidic aqueous electrolytes than organic electrolytes. Thus, this material could be promising for high capacity proton batteries.



ABSTRACT PROPOSAL

Organic Electrode Materials for Magnesium and Solid-state Batteries

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Keywords: *organic electrode materials, rechargeable magneiusm battery, solid-state battery*

ABSTRACT

The clean energy industry is projected to grow rapidly in the coming years, with a heavy reliance on lithium-ion batteries. However, there is a pressing need for innovative battery chemistry that goes beyond lithium-ion, as well as the discovery and design of new materials that can be domestically produced and used to make safe, sustainable, fast-charging batteries at gigawatt scale. This presentation will cover two areas of research. First, we will discuss the development of fast-charging magnesium batteries, which offer advantages over lithium batteries in terms of abundance, domestic availability, and safety. However, multivalent metal-ion chemistries pose technical challenges due to the strong interaction of Mg^{2+} with electrolyte solutions and cathode materials. We will present our work on the development of a highly performing single salt electrolyte and heterogeneous enolization redox chemistry in a Mg battery, resulting in a specific power nearly two orders of magnitude higher than that of state-of-the-art Mg batteries with quick charging capabilities (80% charged within 5 minutes). Second, we will cover the use of organic electrode materials for solid-state batteries, which offer a compelling alternative to inorganic active materials but pose important science questions. We will discuss the design of organic electrode materials with tunable moduli that allow for intimate contact with ceramic electrolytes, moderate redox potential, and high specific capacity via multiple Faradaic reactions per subunit. We will present a novel cathode composite, including pyrene-4,5,9,10-tetraone (PTO) as the cathode in a thiophosphate electrolyte. The implementation of cryomilling enabled the efficient reduction and mixing of the PTO material with the electrolyte, resulting in exceptional material utilization. Finally, we will discuss the pathway to achieve 500 Wh/kg in solid-state batteries using organic electrode materials.

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ABSTRACT PROPOSAL

Investigations of the electrochemical delithiation/lithiation process in magnesium (2,5-dilithium-oxy)-terephthalate

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Keywords: *lithiated organic material, electron diffraction tomography, DFT calculations, electrochemical mechanism*

ABSTRACT

The worldwide Li-ion battery demand raises issues concerning resource availability and recyclability, which are further compounded by the challenges of providing the necessary technical requirements in terms of capacity, cyclability, safety and cost. Therefore, numerous research efforts have been pursued in the quest for alternative chemistries including organic redox. In fact, organic electrode materials offer many interesting opportunities such as design flexibility, lower cost and/or a tempered environmental burden. To date, a myriad of promising electroactive organic materials for application in non-aqueous (metallic) Li- or Na-based batteries have been investigated. However, very few examples of all-organic Li-ion cells have been reported in the literature because of the inherent difficulty in designing efficient lithiated organic cathode materials, as opposed to their inorganic counterparts (e.g., $LiCoO_2$, NMCs or $LiFePO_4$).

A few years ago, our group reported the synthesis and electrochemical performance of magnesium (2,5-dilithium-oxy)-terephthalate (denoted $Mg(Li_2)$-*p*-DHT)[1] as a very promising lithiated positive material able to deinsert/insert lithium ions at 3.45 V vs. Li^+/Li calling for further investigations on this lithiated organic insertion material. In this presentation, we will report on an-going work aiming at elucidating the electrochemical delithiation/lithiation process. This work was made possible thanks to the crystal structure determination of the $Mg(Li_2)$-*p*-DHT compound by using a combination of Precession electron diffraction (PED) and powder X-ray diffraction (PXRD) methods together with DFT calculations. The crystal packing confirms the coordination of Mg atoms to both phenolate and carboxylates groups as anticipated in our first report[1]. In addition, *operando* synchrotron XRD data recorded at the first cycle have demonstrated the reversibility of the electrochemical process in the solid state. The analyses of the collected XRD patterns helped with both DFT calculations and EPR measurements have also enable to propose a structural model for the radical delithiated phase $Mg(Li_1)$-*p*-DHT$^{\bullet}$. An attempt to explain the limitation in capacity to half the theoretical value of this material ($1e^-$/ring against 2 expected) will be discussed too.

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ABSTRACT PROPOSAL

Towards Extreme Capacities for Organic Electrode Materials: Stabilizing Superlithiation Phenomenon

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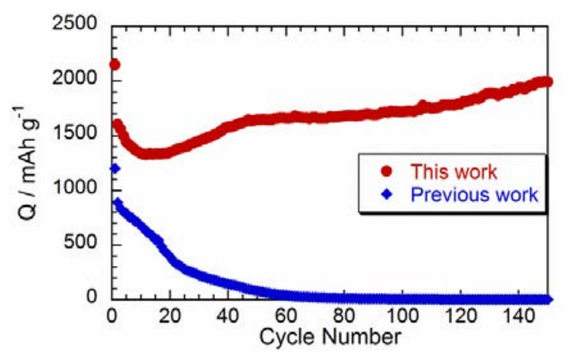
Keywords: *Carboxylates, Superlithiation, Electrode formulation*

The commercial use of organic electrode materials (OEMs) is currently held back, primarily due to their poor energy density. High specific capacity OEMs are therefore of uttermost interest. During the last years, OEMs with the ability of an unexpected reversible reduction of carbon-carbon double bonds have sporadically been reported. As a consequence of this redox process – coined 'superlithiation' – specific energies several times higher than commercial standards (graphite) and Li/C ratios of 1/1 have been reported.

In a previous work on the 'superlithiation' of dilithium benzenedipropiolate [1], we reported that this material can reversibly reduce its unsaturated carbon-carbon bonds in addition to the expected reduction of its carbonyls, leading to a Li/C ratio of 1/1 and specific capacity as high as 1363 mAh g^{-1}: the highest ever reported for a lithium carboxylate. However, the stability of this redox behavior was poor and obvious capacity fading was observed after a few cycles. We here show that better capacity and stability can be achieved with appropriate electrode formulation and optimization of parameters such as calendaring or temperature/electrolyte match (liquid or industrial quality polymer electrolytes).



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AORFB: design, synthesis and integration of organic materials

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Keywords: *AORFB, organic active materials, aqueous electrolytes*

ABSTRACT

Redox flow batteries have been appointed as potential candidates to enable the energy transition. Those open systems present the capability to decouple power and energy and are therefore well suited for stationary energy storage. As in the case of static systems, flow batteries are immersed in the search of abundant materials to meet global energy demand. Vanadium batteries represent the-state-of-the art based on their good performance and stability, and the use of a single active species. Researchers are seeking for alternatives to V_2O_5, listed as a critical raw material.[1]

In this context, organic redox active materials, based on earth-abundant elements have been identified as prime candidates.[2] Molecular engineering would allow to fine tune the properties of active materials in a fit for purpose basis. In the last years, a variety of new compounds have been developed,[1] always with the focus set on the solubility and the redox potential of the compounds, which ultimately define energy density of the system. Only very recent studies have put the focus on the stability of the active materials and their integration into the electrolyte.

The challenges in the development of electrolytes from active material design to solution formulation are presented with practical examples.

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ABSTRACT PROPOSAL

Unprecedent Capacity of non-functionalized TEMPO Catholyte and their application in Aqueous Redox Flow Batteries

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Keywords: *organic redox flow battery, TEMPO, viologen*

ABSTRACT (200 words max.)

Redox flow batteries (RFB) are a unique type of batteries which allows decouple power and energy making them promising candidates for large-scale energy storage applications1. Recently, organic redox active compounds have been considered as sustainable alternative to replace the currently used vanadium active species. The low solubility of the non-functionalized TEMPO in water (≈70 mM) has hindered the application of this interesting redox active species in aqueous RFBs to date.

In our research, we report a simple approach to solubilize large amount of pristine TEMPO in aqueous solution reaching an unprecedented solubility (up to 5.6 M in presence of supporting electrolyte), corresponding to a theoretical volumetric capacity as high as 150 Ah/Lcatholyte. Our approach consists on modifying the properties of the supporting aqueous electrolyte to promote intimate interaction between supporting salt and pristine TEMPO.

The electrochemical performance of this TEMPO catholyte was excellent with a fast kinetics (k^0 = 0.018 cm/s) and impressive long-term stability in symmetric RFB configuration (0.552%/day). This new TEMPO catholyte was paired with a sulfonated viologen anolyte resulting in a RFB with a theoretical energy density of 22.15 Wh/L, an open-circuit voltage of 1.08 V and very low capacity fading over cycling (0.60%/day and 0.048%/cycle).

Organic Battery Days 2023
June 7-8th, Donostia-San Sebastián

ABSTRACT PROPOSAL

Data Science based Electrolyte Design for Organic Redox Flow Batteries

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Keywords: *Redox Molecule Design, Machine Learning, Redox Flow Battery, High throughput Robotics*

ABSTRACT

Ability to design materials for targeted functionality rather than traditional intuitive and trial-by-error based methods can bring enormous societal and technological progress. In this context, exploring the large space of potential materials for energy storage device is computationally intractable. In particular, the discovery of organic redox active species - which dictates the energy density, specific capacity and cycle life is critical step in realizing viable redox flow battery (RFB) technology - will be taunting challenge considering billions of organic structural possibilities. Traditional methodology relies on combinatorial approach of additives, functional groups, and solvent composition to achieve higher solubility and stability of the specific redox molecule. However, considering the wide range of materials selection, it is imperative to build an artificial intelligence-based design formulation that will help us bottom-up design of RFB electrolytes. This framework helps us in solvent and functional group selection process, and ultimately enhance the solubility and stability through inverse design of redox active molecules. We will discuss our efforts and recent results related to the data science-driven and high throughput robotics validated electrolyte design formulations applicable for organic molecule based redox flow battery systems.

ABSTRACT PROPOSAL

Self-healing binders with boron-based linkers

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Keywords: *self-healing binders, dynamic covalent bonds, boronic esters, silicon electrodes*

ABSTRACT (200 words max.)

The use of self-healing materials in battery applications is rapidly increasing. Among the variety of bonding types, hydrogen bonds are the most widely explored because they can form and break easily thanks to their weak interactions. Nevertheless, this could also be a disadvantage as this high reversibility could render poor mechanical properties desired for their intended application.

An alternative solution is to use dynamic covalent bonds which are also reversible, thus allowing self-healing properties, whilst having higher bonding strength and mechanical stability. Many battery materials would benefit from improving their mechanical strength, especially those suffering from large volume changes and cracking during cycling, such as silicon.

Herein, we present the use of dynamic covalent bonds as self-healing binders for silicon electrodes. They are based on poly(vinyl alcohol) (PVA) and boron-based linkers. Electrodes containing these self-healing binders show improved electrochemical performance compared to the reference PVA binder. Furthermore, we shed some light on the self-healing reaction mechanism and the effect that these new functionalities have inside the electrochemical cell.

ABSTRACT PROPOSAL

ORGANIC ELECTROACTIVE BASED AQUEOUS ION-BATTERIES FOR ENERGY STORAGE AND WATER DESALINATION

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Keywords: *aqueous ions battery, zinc, energy storage, water desalination*

ABSTRACT (200 words max.)

Aqueous ion-batteries such as zinc-ion systems integrating organic active materials[1], stand out as highly promising contenders for stationary electrochemical storage while limiting environmental footprints. However, many organic molecules are prone to dissolution in aqueous electrolytes. Several strategies have been proposed to overcome this limitation such as polymerization[2] and design of macrocycle[3] which both require multi-steps synthesis. Solubility of small molecules can also be limited by using high symmetry monomers with low dipole moments[4] or inter-molecular H-bonding[5]. Herein we will present an alternative low cost material family and describe its electrochemical and physical properties using various electrolyte chemistries. This talk also reports on organic material search for water desalination.

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Polymer-based redox flow batteries and solid-state polymer batteries

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The efficient storage of electric energy represents a major challenge for a successful energy transition, enabling the utilization of fluctuating renewable resources also as base load. Redox-flow-batteries (RFBs) are the only type of battery where intrinsically power and capacity can be varied independently from each other, making this type of battery perfectly suited for scalable stationary applications.

RFBs based on aqueous electrolytes with organic / polymer active materials have the potential to be suitable alternatives for commercial metal-based RFBs, with low CO_2 footprint perfectly fitting to the goals of the EU Green Deal.

In particular, polymer-based RFB systems enable the use of cost-efficient dialysis membranes together with pH neutral table salt solutions as electrolytes.

The lecture will discuss the current status of the polymer-based battery systems explored in Jena, Germany.

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ChemSusChem **2023**, *in press*, e202300296 (doi: 10.1002/cssc.202300296)

ABSTRACT PROPOSAL

INTRODUCING SMART FUNCTIONALITIES IN SOLID POLYMER ELECTROLYTES

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Keywords: *solid polymer electrolytes, liquid crystals, vitrimers, fire-retardant properties self-healing*

ABSTRACT

Nowadays, batteries are mainly using the lithium-ion technology with its inherent drawbacks including the use of organic solvents-based electrolytes, the impossibility to reach a high voltage (>4.5V vs Li^+/Li) and the need to significantly improve the energy density. To face these issues, the technology of all solid state lithium metal batteries is currently investigated. Indeed, the utilization of a lithium metal anode is the most obvious way to increase the energy density. However, due to the high reactivity of lithium metal and the need to create a stable solid electrolyte interface (SEI), this new generation of batteries requires new innovations regarding the electrolytes. In this respect, solid polymer electrolytes (SPEs) are interesting candidates. The ideal SPE must be compatible with both lithium metal anodes and with high voltage cathode materials (until 5 V vs Li^+/Li) and with all the materials contained in both electrodes. Its ionic conductivity at room temperature must be beyond 0.1 mS/cm in order to allow the battery to deliver an adequate power density compared to liquid electrolyte. Lastly, it should offer good mechanical properties (modulus > 6 GPa) to avoid dendrites growth, and be easily processable.
Based on those considerations, we report here novel SPEs integrating smart functionalities. Those include fire-retardant properties provided by phosphonate moieties, self-healing properties provided by the introduction of covalent dynamic bonds in vitrimer-like SPE, and oriented lithium-ion conduction channels for improved ion transfer in liquid-crystalline SPEs.

ABSTRACT PROPOSAL

Addressing Practical Use of Viologen-Derivatives in Redox Flow Batteries through Molecular Engineering

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Keywords: *redox flow batteries, viologen-derivatives, capacity fading, chemical degradation,*

ABSTRACT

Redox Flow Batteries (RFBs) are promising energy storage systems for stationary energy application, which are featured by their independent scalability of energy and power. All Vanadium flow batteries represents the state-of-the-art RFBs. However, vanadium is a critical materials for the USA and the EU, so that substitution of vanadium species by highly soluble organic redox species is gaining interest. In neutral pH, viologen derivatives are the most widely used and studied organic species for the negative side due to their redox potential and solubility. Unfortunately, in practical scenarios, viologen-derivatives face an accelerated degradation in the unavoidable presence of traces of oxygen in large-scale RFBs.

Herein, we evaluate the primary degradation mechanism and propose a straightforward, cheap, and fast method to evaluate the stability of viologen-derivatives towards this degradation. Considering that the cleavage of the N-substituent is the main proposed pathway for viologen degradation, a new viologen-derivative, bearing an alkylsulfonate chain with a secondary carbon centre joined to the N atom, is synthesized to illustrate how molecular engineering can be used to improve stability. By introducing a hysterical impediment, chemical degradation is reduced leading to a 3-folds decrease in capacity fading.

ABSTRACT PROPOSAL

Discovering redox-stable organic battery electrodes using AI

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Keywords: *artificial intelligence, materials discovery, organic electrode, alkali-metal battery, redox stability*

ABSTRACT

Data-driven approaches have been revolutionizing materials science and materials discovery in recent years. Especially when coupled with other computational physics methods, they can be applied in complex high-throughput schemes to discover novel materials, e.g. for batteries. In this direction, we have developed a robust AI-driven framework, to accelerate the discovery of novel organic-based redox-active potential cathode materials. Recently, we have extended this to involve both Li-, Na- and K-ion batteries. The platform is able to predict the open-circuit voltage of the respective battery, but also to provide an initial assessment of the materials redox stability – a ciritical parameter which has been negelcted in previous aproaches. The kernel was employed to screen 45 million organic molecules in the search for novel high-potential cathodes, resulting in a proposed shortlist of only a few thousands or hundreds of novel compounds for Li-, Na- and K-ion batteries, respectively. Thereby, the chemical space has been clearly limited, while there are also several suggestions for new compounds.

ABSTRACT PROPOSAL

Improvement in current collecting property of organic positive electrode and its electronic conduction mechanism

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Keywords: *Quinone, High-energy density, Practical electrode design.*

ABSTRACT (200 words max.)

Aiming to increase the capacity and energy density of rechargeable lithium batteries, we have been studying organic active materials with high capacity per weight. Since organic active materials have low electronic conductivity, it is often necessary to use a large amount of conductive additives to achieve a capacity close to the theoretical value. Addressing this issue, and found that using CNTs as a conductive additive and adjusting the size of the active material particles is very effective. Even when the ratio of an active material (a naphthazarin dimer) in the electrode is more than 90%, sufficient capacity was obtained. Furthermore, scanning spreading resistance microscopy (SSRM), which can monitor the resistance of the electrode, revealed that the resistance of the active material decreases rapidly during the charge/discharge process.

These results indicate that it is possible to increase the organic active material ratio to the level of practical batteries, and that the problem of current collecting properties of organic batteries, which had been considered intrinsically difficult, can be overcome through electrode design.

Abstracts for Flash and Poster Presentations

ABSTRACT PROPOSAL

Robust Aluminum//Phenazine Conjugated Porous Polymer Metal-Organic Batteries

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Keywords: *phenazine-based battery, Al-organic battery, Conjugated porous polymer*

ABSTRACT (200 words max.)

Rechargeable aluminum metal batteries (RAMBs) are an electrochemical energy storage technology that hold great promise for large-scale applications owing to the high natural abundancy of Al, cost-effectiveness, safety and sustainability. Up to date, the most diffused RAMBs are constructed using graphite or inorganic intercalation/conversion cathodes as transitional metal oxides; however, the first battery features low energy density while the second one suffers from poor kinetics and short cycle-life due to inevitable volume expansion/contraction during battery operation.[1] One of the possible solutions to circumvent the sluggish kinetics, low capacity and poor integrity of inorganic cathodes might be the use of organic electrode materials (OEMs). OEMs not only feature structure tunability and sustainability but are also characterized by a unique ion coordination mechanism that makes them universal charge carriers hosts.

Here, we present a new phenazine-based hybrid microporous polymer developed by our group (IEP27-SR) [2] as organic cathode in ionic liquid electrolyte ($AlCl_3$/EMIMCl) for Al-metal battery. The introduction of phenazine active units into a robust porous framework resulted in an impressive capacity retention even at high current densities (80% retention at 10C with 90 mAh/g) and a remarkable cycle stability even after 130 days of cycling (3500 cycles, 77% of retention at 1C) sustaining 75 mAh/g.

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Organic Battery Days 2023
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ABSTRACT PROPOSAL

Bio-based Polyhydroxyanthraquinone Redox Polymers as High-Voltage Organic Cathode Materials for Lithium-Ion Batteries

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Keywords: *Organic Cathode Materials, Small molecules, Polymers, Bio-based, High-voltage, Lithium-ion Batteries*

ABSTRACT (200 words max.)

Despite still being the state-of-the-art battery chemistry for many applications, the predicted high deployment numbers of Lithium-Ion Batteries raises various environmental concerns related to the scarcity, topographical limited harvesting and energy intensive mining and processing of crucial inorganic electrode materials such as nickel, cobalt and manganese. As a sustainable alternative, Organic Electrode Materials (OEMs) have been proposed as promising alternative due to their modifiable organic structures, abundancy and energy efficient processing. [1-3] Although multiple materials show impressive capacities, OEMs exhibiting high redox potentials (>3.5V vs. Li/Li^+) remain scarce and many starting materials are still derived from the fossil fuel feedstock. [4,5]

In this work, we present a set of high-voltage, bio-based polyhydroxyanthraquinones and their polymer counterparts as high-voltage cathode materials for LIBs. Dependent on the molecular structure, the high-voltage discharge potentials are typically between 3.8-4.2V with initial specific capacities of up to 383 mAh g^{-1}. Furthermore, we show that a facile polymerization process, utilizing formaldehyde as linker and MWCNTs as scaffolds, improved the cyclability of the materials, retaining the high discharge potential starting at 4.0V (vs. Li/Li^+) and capacities as high as 81.6 mAh g^{-1} after 100 cycles when utilizing both the catechol like moieties and the anthraquinone functionality.

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ABSTRACT PROPOSAL

A holistic approach to the design of practical polymer organic batteries

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Keywords: *organic battery, redox polymer, PTMA, simulation*

ABSTRACT (200 words max.)

Redox polymer-based organic batteries have emerged as a potential sustainable, low-cost, and safe alternative to lithium-ion batteries.[1] One of the most studied and promising organic electrode materials is poly(2,2,6,6-tetramethyl-1-piperidinyloxy methacrylate) (PTMA), which belongs to the p-type class.[2] However, designing practical batteries with PTMA requires careful consideration due to the redox mechanism involving the anions in the electrolyte and the low electronic conductivity of polymers as cathodes.[3]

The synthesized active material, a mixture of PTMA and multiwalled carbon nanotubes, was used as cathode in lithium metal batteries.[4] With simple aqueous processing, high active mass loading electrodes between 4.2 and 9.6 mg·cm^{-2} were obtained, among the highest reported for lithium-based systems (Figure 1). These experimental results were critically evaluated with a novel physical model and a cost and energy density analysis software. With optimistic hypotheses on the battery design, the cost of a PTMA battery could compete with lithium metal batteries with inorganic cathodes, but the energy density would remain nevertheless much lower.

In summary, lab-scale coin cells showed good results, but simulations revealed the challenges of translating these performances into real-world applications, highlighting the need for accurate electrode engineering and the use of superconcentrated electrolytes to achieve practical PTMA batteries.

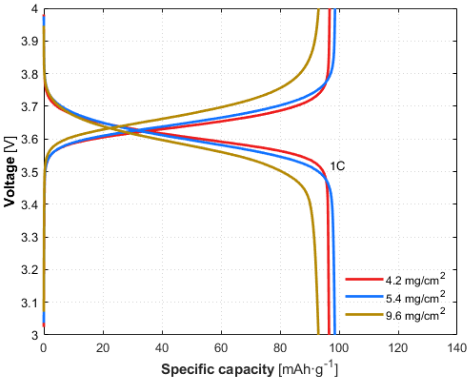

Figure 1 - Voltage/capacity curves at 1C for three PTMA|Li coin cells with the same electrode composition and different mass loadings

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Liquid crystals as additives in solid polymer electrolytes for lithium metal batteries

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Abstract

The forefront of research for new electrolyte materials for tomorrow's electrochemical energy storage technologies is based on thoroughly designed molecular architectures. Here, liquid crystals (LCs) mixed with poly(ethylene-oxide) (PEO) and lithium salts are proposed as solid polymer electrolytes (SPEs) for application in lithium-metal batteries. The PEO matrix comprises the LC, which gives orientational properties, whereas the PEO chains with lithium salts are responsible for the ionic conductivity. N-(4-Methoxybenzylidene)-4-butylaniline (MBBA) is used as proof-of-concept and new LC molecules are developed for further research. The resulting SPE is shown in Figure 1 Ionic conductivities ($7 \cdot 10^{-4}$ $S \cdot cm^{-1}$ at 40 °C) up to three times higher than the reference without LC are achieved. In addition, the SPEs are characterized electrochemically, thermally and by polarized optical microscope demonstrating the preservation of the liquid crystalline behavior even after mixing with PEO and lithium salts.

Figure 1: Picture of solid polymer electrolyte membrane based on PEO with LC as additive.

ABSTRACT PROPOSAL

PDADMATFSI-Poly(Vinyl Benzoate) Triblock Copolymers for Sodium Metal Battery Applications

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Keywords: *sodium, solid-state polymer electrolyte, Na metal batteries, Na-O_2 batteries*

Because of the great abundance of sodium (Na) and rising cost of lithium (Li), Na batteries have long been recognized as a potential alternative to Li batteries. Sodium metal batteries are still a novel research field and many issues regarding this technology has yet to be overcome, and a fundamental component to address the drawbacks of sodium-based batteries is an electrolyte that can prevent major problems, like dendrite formation.[1] One category of materials for overcoming the drawbacks of sodium-based technologies are solid polymer electrolytes (SPEs). among this category of materials, polymerized ionic liquids (PILs) are particularly promising, when compared to typical PEO systems.[2,3]

In this study, we look at a block copolymers (BCP) based on a poly(vinyl benzoate)-b-poly(diallydimethylammonium)bis(trifluoromethanesulfonyl)imide-b-poly(vinyl benzoate) (PVB-b-PDADMATFSI-b-PVB). Different formulations of PVB-b-PDADMATFSI-b-PVB were synthesized, investigating the influence of chain lengths of the two co-monomer (PVB and PDADMATFSI) on the physiochemical properties of the BCP. The best formulation was selected to be mixed with NaFSI and obtain a self-standing SPE membrane. The resulting membranes achieved a conductivity of 10^{-5} S cm^{-1} at 50°C at a concentration DADMATFSI:NaFSI 1:2 mol ratio. The membranes were applied in sodium metal batteries, in particular sodium-oxygen batteries (SABs), achieving a discharge capacity of 1.2 mAh cm^{-2}, which results competitive to the state-of-art solid state SABs.[4,5]

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ABSTRACT PROPOSAL

Multivalent Ion Transport in Organic Electrodes: A Microscopic Study

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Keywords: *Electron microscopy, multivalent batteries, organic cathodes*

ABSTRACT (200 words max.)

Rechargeable batteries based on energy-dense multivalent metal anodes (such as Mg and Ca), could represent a major step forward in the transition to a renewable energy economy. When paired with organic cathodes with weak intermolecular forces, multivalent metal batteries could reach their full potential. One of the main problems organic materials face when coupled with Mg or Ca ions is a sharp decrease in active materials utilization, compared to the values obtained in Li half-cells.

In order to understand the origin of this inferior performance, in this work, we provide a comprehensive microscopic study on model poly(anthraquinonyl)sulfide polymer cycled inside Mg and Ca cells. Obtained results were interpreted in conjunction with electrochemical impedance spectroscopy data to help understand the origin of ion diffusion limitations in organic materials. Insights gained can be used for directing future polymer designs that would allow for better utilization when coupled with multivalent charge carriers, leading to efficient energy storage technology of the future.

ABSTRACT PROPOSAL

(Metal-)Organic Battery based on PANI/Polycatechol Hybrid

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Keywords: *organic electrode, polycatechol, polyaniline, zinc battery*

ABSTRACT (200 words max.)

The importance of developing safer, greener and more sustainable batteries has increased due to the rising demand for environmentally friendly technologies and clean energy ambitions. These batteries are designed to minimize the negative impact of traditional batteries on the environment footprint by utilizing eco-friendly materials and production techniques. Our study introduces a facile approach for synthesizing a conductive polymer-redox polymer hybrid electrode via counter ion exchange[1]. In this reaction, different weight ratios of Polyaniline (cationic polyelectrolyte) and Poly(VC-co-SS) (anionic polyelectrolyte) [2] reacts together to form a hybrid polymer material which is then employed in zinc or all-organic batteries. Specifically, electrodes with different ratios of PANI/Polycatechol are synthesized and employed as organic cathode in Zinc batteries using Zn metal as anode and all-organic proton battery using an appropriate polymer anode. This reaction is anticipated readily scalable and possibly holds the potential to decrease the carbon content (typically down to 10s wt%) in current electrodes, thus enhancing energy density at the electrode level and could promote the development of more sustainable electrodes for scalable applications.

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ABSTRACT PROPOSAL

DESIGN OF NOVEL TYPES OF HYBRID POLYMER/INORGANIC SOLID ELECTROLYTES WITH ENHANCED IONIC CONDUCTIVITIES

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Keywords: *hybrid electrolytes, flame-retardant, lithium metal battery*

ABSTRACT (200 words max.)

Abstract text
Hybrid polymer/inorganic solid electrolytes have been considered one of the promising routes toward improved safety and higher energy density compared to today's liquid electrolytes. Herein, flame-retardant phosphorus-containing random copolymers, namely poly(oligo(ethylene glycol) methyl ether methacrylate)-co-(dimethyl(methacryloyloxy)methyl phosphonate) (P(xPEGMA-co-yMAPC1)), are synthesized with different monomer compositions. The solid polymer electrolytes are obtained by mixing P(xPEGMA-co-yMAPC1) with lithium perchlorate ($LiClO_4$) and acetonitrile (ACN). Among the copolymer electrolytes, the P(9PEGMA-co-1MAPC1) with 10wt% $LiClO_4$ presents a good flame-retardant performance and exhibits an ionic conductivity of 1.0×10^{-4} S cm^{-1} at 60°C. To further enhance the ionic conductivity of the copolymer electrolytes, hybrid polymer/inorganic solid electrolytes are synthesized by adding $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) and SiO_2 inorganic fillers, respectively. P(9PEGMA-co-1MAPC1) with 10wt% LATP exhibits a higher ionic conductivity of 1.4×10^{-4} S cm^{-1} at 60°C, while the sample with SiO_2 fillers shows similar ionic conductivity. Finally, the cycling performances of hybrid solid electrolytes containing $LiFePO_4$|P(9PEGMA-co-1MAPC1) + $LiClO_4$+LATP/SiO_2|Li batteries have been tested. The capacity reaches 164.2 mAh g^{-1} at 0.05 C, and the capacity retention reaches 90% after 200 cycles at 0.1 C.

ABSTRACT PROPOSAL

Polyrotaxane-based networks as electrolytes and catholytes for all solid-state lithium batteries

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Keywords: *Polyrotaxane, Solid polymer electrolyte, Catholyte, All solid-state lithium battery*

ABSTRACT

All solid-state lithium batteries are becoming increasingly noticeable in recent years due to their excellent properties such as high energy density and high safety. Selecting the suitable polymer materials used as solid polymer electrolytes (SPEs) and the catholytes is crucial for improving the electrochemical performance of all solid-state lithium batteries. Acordint to the different requirements for SPEs and the catholytes, two polyrotaxane-based networks, CPR500 and CPR2000, have been prepared, loaded with lithium salts and further used as SPEs and cathoclytes for all solid-state lithium batteries. The networks were obtained from polyrotaxanes functionalized by poly(ethylene glycol) diglycidyl ether (Mn=500 and 2000). The polyrotaxanes were composed of many macrocycles (α-cyclodextrins, α-CD) threaded onto a linear poly(ethylene glycol) (PEG) chain end-capped at both ends with bulky stoppers. The CPR500-$LiClO_4$ SPE shows a high ionic conductivity of 7.25×10^{-4} S cm^{-1} and a wide electrochemical stability window from 1.6 to 4.0 V at 60°C. CPR500-$LiClO_4$ shows the better interfacial stability with lithium metal than that of PEO-$LiClO_4$. When CPR2000-$LiClO_4$ is used as catholyte in $LiFeO_4$ cathode (LFP2000) and lithium metal is employed as anode, the LFP2000||CPR500-$LiClO_4$||Li cell can achieve a high initial capacity above160 mAh g^{-1} at 0.1 C (60°C).

ABSTRACT PROPOSAL

A novel fluorinated alkoxyaluminate-based electrolyte for Ca batteries

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Keywords: *Ca batteries, electrolyte, fluorinated alkoxyaluminate, oxidative stability, organic cathode*

ABSTRACT

Ca batteries are considered as promising post-Li energy storage systems due to the bivalent nature of Ca ion, low redox potentials, high gravimetric capacities, and natural abundance. The main challenge remains the lack of suitable electrolytes, enabling reversible stripping and plating of Ca metal. A few years ago, fluorinated alkoxyborate-based electrolytes were introduced to Mg and Ca batteries and surpassed the previous generations of electrolytes by displaying lower overpotentials and Cl-free character. Recently, additional electrochemical performance improvement has been achieved with a substitution of borate with aluminate electrolytes for Mg batteries, which motivated our research.

A synthesis procedure for a novel $Ca[Al(hfip)_4]_2$ salt was developed and salt was benchmarked versus state-of-the-art boron analogue $Ca[B(hfip)_4]_2$. New aluminate-based electrolyte exemplifies better performance in terms of ionic conductivity, Ca plating/stripping efficiency, and oxidative stability. Additionally, we compare the performance of both electrolytes in a Ca metal anode-organic cathode cell setup, using naphthalene-hydrazine diimide polymer as a cathode material. The research exposes the appealing properties of $[Al(hfip)_4]_2^-$-based electrolytes and their potential for future investigation in different batteries.

ABSTRACT PROPOSAL

Development of Advanced All-Solid-State Polymer Electrolytes Using Innovative, Rapid, and Solvent-Free Procedures

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Keywords: *Lithium-ion batteries, Solid-state electrolytes, Hybrid ionogels, Methacrylic monomer(s), Room temperature ionic liquids.*

ABSTRACT (200 words max.)

Solid-state electrolytes (SSEs) aim to overcome the safety issues, to decrease the package volume and to increase the energy density of next-generation energy storage devices.[1] The ion gel (or ionogel) systems, in which room-temperature ionic liquids are doped within a solid matrix, are amongst the most attractive.[2] Here, we present the results of methacrylate-based SSEs including organic and organic–inorganic hybrid/composite materials conceived for ambient temperature cycling with high-energy cathodes. This work sheds light on the design and development for the safe electrolyte system towards all-solid-state batteries.

Acknowledgement: This work has received funding from the EU Horizon 2020 programme under the Marie Skłodowska-Curie grant agreement No 860403.

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ABSTRACT PROPOSAL

NOVEL ORGANIC CATHODE MATERIALS BASED ON PYRAZINE AND QUINONE MOTIFS FOR RECHARGEABLE LITHIUM-ION AND ZINC-ION BATTERIES

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Keywords: *organic, cathode, zinc, lithium*

ABSTRACT (200 words max.)

Despite numerous reports on novel small organic cathode materials (SMOC) for rechargeable lithium-ion and zinc-ion batteries, there is still a lack of materials that exhibit satisfactory cycling stability. For their use in large scale energy storage systems, it is desired that the materials are derived from commercially available precursors through facile synthesis. Recently, several studies showed that the incorporation of quinone and pyrazine units into organic cathode materials could simultaneously increase the voltage and capacity of materials. Herein, we present several novel SMOCs based on quinone and pyrazine redox active motifs. Novel materials are derived from hexaazatrinaphthalene (HATN), a small organic cathode material, of which derivatives have already been explored as positive electrode materials in zinc-ion and lithium-ion batteries delivering high specific capacities. We synthesized a novel HATN based small organic cathode materials derived by a synergistic combination of hexaazatriphenylene (HAT) core and different quinone motifs enabling increased theoretical capacities up to 669 $mAhg^{-1}$. We will present a facile synthesis strategy, which enables the simultaneous incorporation of pyrazine and quinone units in one step synthesis from commercially available precursors yielding materials with high capacities and cycling stability.

ABSTRACT PROPOSAL

High performance coordination polymers for post-Li battery technologies

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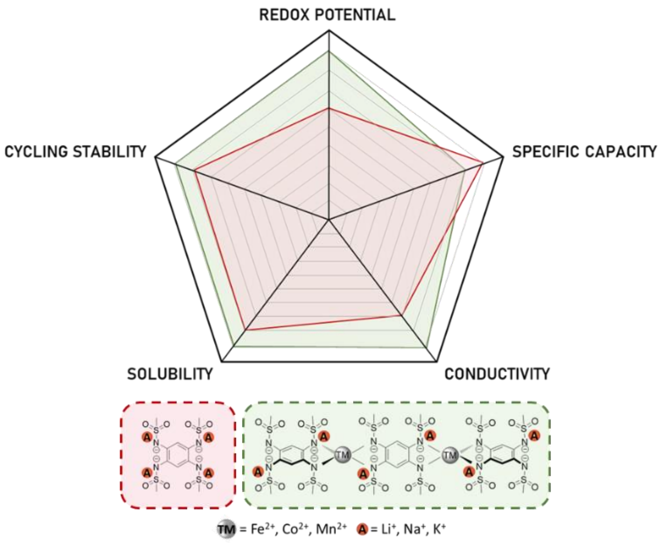
Keywords: *coordination polymer, conjugated sulfonamide, cathode material, post-Li batteries*

ABSTRACT (200 words max.) **preferably for a talk**



Due to the ever-increasing demand for energy and the limited available resources, the interest for post-Li technologies has been growing considerably in recent years[1]. Among the developed technologies, organic battery materials constitute more efficient and robust tools toward post-Li cation storage compared to their inorganic analogues. However, the development of cation reservoir and high voltage operating organic materials still remains a huge challenge in the field. Herein, we report a high voltage alkali cation containing coordination polymer, with the generic formula of A_2-TM-PTtSA (wherein A = Li^+, Na^+, or K^+; TM = Fe^{2+}, Co^{2+}, or Mn^{2+}), based on a benzene-1,2,4,5-tetrayltetrakis methylsulfonyl-amide (PTtSA) reversible redox centre[2]. We demonstrate that using a coordinating cation centre (TM) drastically increases the average redox potential to 2.95–3.25 V for Li-, Na- and K-ion batteries, and leads to an increase in electrical conductivity of even two orders of magnitude compared to A_4-PTtSA. Finally, we found that the reported coordination polymers are insoluble in battery electrolytes, have high gravimetric density, and can be cycled with low carbon content and high mass loading.

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ABSTRACT PROPOSAL

Novel Organic Redox-Active Compounds for Next Generation Redox Flow Batteries

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Keywords: *energy, redox flow, organic.*

ABSTRACT (200 words max.)

Redox-flow batteries have emerged as relevant candidates for large-scale stationary energy storage, owing to their unique capability to decouple energy storage and power generation.

Recent developments have witnessed a transition from inorganic redox-active materials to water-soluble organic compounds, which offer low cost, high sustainability, and structural diversity.

In recent years, acidic, alkaline, and neutral AORFBs using different organic molecules/polymers as redox-active materials have been explored.

In the pursuit of more sustainable and cost-effective batteries, the substitution of acid and alkaline electrolytes with gentler alternatives is a crucial aspect to consider.

Among the compounds investigated in the literature, OH-TEMPO has emerged as the most promising candidate. Nevertheless, its practical implementation is hampered by stability issues or complex synthetic processes.

In this context, we have contributed to the development of novel nitroxyl radicals that exhibit superior solubility in aqueous solutions at neutral pH and higher redox potentials. Our study presents a significant contribution to the advancement of neutral pH AORFBs by introducing a novel anolyte-catholyte combination.

We have conducted a comprehensive study on the Viologen-TEMPO based electrolyte, which includes synthesis, characterization, and battery testing. Our findings offer valuable insights into the potential of this novel technology for practical applications.

ABSTRACT PROPOSAL

PDDAFSI-PYR13FSI-LiFSI-LLZO hybrid electrolytes for high-voltage solid state lithium metal batteries

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Keywords: *Solid state battery, Lithium metal battery, Hybrid electrolytes, High voltage cathode*

ABSTRACT

Solid-state lithium metal batteries (SSLMBs) are considered to be a promising next-generation energy storage solution due to high energy density, enhanced safety and improved durability. However, one of the primary challenges in developing of SSLMBs is finding solid polymer electrolytes (SPE) with improved electrooxidation stability compatible with high-voltage cathodes such as Ni-rich NMC. This has led researchers to search for new polymeric materials that can overcome this limitation. One such polymer is poly(diallyldimethylammonium bis(fluorosulfonyl)imide) (PDDA-FSI), which has shown promising results when combined with an ionic liquid.

Hence, in this study a SPE was prepared using PDDA-FSI as the polymeric matrix, together with $PYR_{13}FSI$ and LiFSI. The prepared SPE based on the ternary gel has a high ionic conductivity of $6.0x10^{-4}$ S/cm at 25°C. However, it demonstrates poor mechanical properties especially at high temperature (>50ºC).

To address this issue, different quantities of $Li_{6.24}La_{3}Zr_{2}Al_{0.24}O_{11.98}$ (LLZO) filler single ion property were added to the SPE to improve the mechanical and electrochemical properties. The PDDAFSI-PYR13FSI-LiFSI-LLZO hybrid electrolytes show better mechanical properties and achieve a good ionic conductivity of $2.7x10^{-4}$ S/cm at 25°C. They were also tested in symmetrical Li-Li and $Li/LiNi_{0.6}Mn_{0.2}Co_{0.2}O_{2}$ solid state coin cells. More experimental results will be provided in the poster.

ABSTRACT PROPOSAL

AN ECODESIGNED CARDBOARD PRIMARY BATTERY FOR SMART PACKAGING APPLICATIONS

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Keywords: *Ecodesign, alternative batteries EoL, portable power sources, paper/cardboard recycling*

ABSTRACT

Batteries have become an essential power source, due to their capability to deliver high energy densities in a portable manner. Although secondary batteries seem to be the most prominent solution, many applications in which logistics requirements make battery recovery very unlikely, rely on primary non-reusable options. A close look into batteries life cycles reveals an obsolete linear model, which still relies on scarce non-renewable resources with environmentally unsatisfactory collection rates and recycling systems. The current situation sets a great opportunity for re-thinking portable batteries' life-cycle under an environmentally conscious framework.

This work presents a primary battery envisioned for smart-packing applications, which redefines the conventional battery life cycle through ecodesign. Material exploration and selection of low energy-consuming fabrication methods are essential to minimize the power source-associated environmental impact. Herein current collectors are generated via Laser-Induced Graphene over pre-treated cardboard. Bio-polymers, synthesized from naturally occurring polymers, are used to create hydrogels that retain the redox species and act as ion exchange membranes. Their unique composition allows the battery to be recycled with cardboard, readily aligning the battery's end-of-life with the application. The battery concept presented showcases a feasible pathway to develop truly sustainable portable energy storage device alternatives.

ABSTRACT PROPOSAL

Investigating Bio-derived Polyhydroxy urethanes network bearing carbonates as solid polymer electrolyte

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Keywords: *Electrolytes, bio-based, Lithium batteries*

ABSTRACT

Climate change is a harsh but ultimate reality, impacting every corner of the globe. This stresses the strong emphasis on the need for clean renewable energy with safe storage technology, particularly batteries. Solid-state batteries are of great interest owing to their higher energy density, flexibility and safety than the existing lithium-ion batteries technology. While there is constantly increasing research on polyethylene oxide (PEO) based polymers, we aim at PEO alternatives that are sustainable and environmentally friendly. In our project, we demonstrate a bio-derived solid polymer electrolyte based on functionalized carbonated soybean oil (CSBO) monomer for the synthesis of polyhydroxy urethanes (PHUs) network. This class of materials shows remarkable adhesive properties on the surface of lithium speculating better interfacial contact and stability. All these polymers reinforced with LITFSI were characterized following standard electrochemical measurements exhibiting decent ionic conductivity (>10^{-2} mS cm^{-1}), electrochemical stability window (> 4 V vs Li/Li^{+}) and transport properties allowing them to be explored for commercial cathodes like $LiFePO_4$. We hope to provide a promising direction for developing bio-derived solid electrolytes to facilitate progress in a sustainability, cost-effective and safe manner towards solid-state lithium battery for global utilization.

Self-Organized High-Energy Organic Electrodes

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Keywords: *Self-organization, electrode engineering, packing density, anode, organic lithium battery*

ABSTRACT

Organic active materials (OAMs) are providing the potential to realize truly sustainable batteries for, e.g., wearables or stationary storage.[1] However, the eventual realization of commercially meaningful electrodes based on such materials still faces several challenges, including the electrode density and areal capacity.

Herein, we propose exemplarily for tetra-lithium perylene-3,4,9,10-tetracarboxylate a multiscale self-assembly-derived electrode engineering to achieve high mass loading organic electrodes with an exceptional electrode density of 1.0 g cm^{-3} and very high areal capacity of 3.4 mAh cm^{-2}. The carefully designed electrode microstructure including highly ordered and interconnected channels for the electrolyte and the well-organized OAM particles along with the electron-conducting additive guarantee efficient charge transport, even in ultra-thick organic electrodes. This strategy will facilitate the development of commercially viable organic electrodes for more sustainable rechargeable batteries.

Reference

[1] Y. Lu et al., Nat. Rev. Chem. 4, 127–142 (2020).

ABSTRACT PROPOSAL

Low-cost and sustainable aqueous lithium-ion batteries by all-organic PTCDI anodes

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Keywords: *lithium-ion battery, organic, aqueous electrolyte*

ABSTRACT (200 words max.)

Water-in-salt electrolytes (WiSEs) has enabled aqueous lithium-ion batteries (ALIBs) to cycle well and to operate at potentials beyond the electrochemical stability window of water. WiSEs are, however, intrinsically based on high concentrations of salt(s) which furthermore often are expensive and fluorinated, and therefore defeats the aim of ALIBs being low-cost and sustainable. Strategies to circumvent this issue have been to add co-solvents and/or diluents to decrease the overall electrolyte concentration or customize the anion and salt concentration to each battery chemistry. The clean and green ethos of ALIBs can be enhanced by using organic active materials (AMs), but these are unfortunately often water soluble and therefore requires an electrolyte designed to mitigate dissolution/electrode de-attachment.

Herein, we for the first time implement perylene-3,4,9,10-tetra-carboxylic-di-imide (PTCDI) as the anode AM for ALIBs. We demonstrate that by appropriate aqueous electrolyte selection se can truly mitigate electrode de-attachment, leading to excellent properties in terms of capacity, rate capability, cycling stability, and Coulombic efficiency. All things considered, this endeavour intends to further reduce the kWh/€ and thereby reinforcing the feasibility of more cost-effective large-scale battery energy storage solutions.

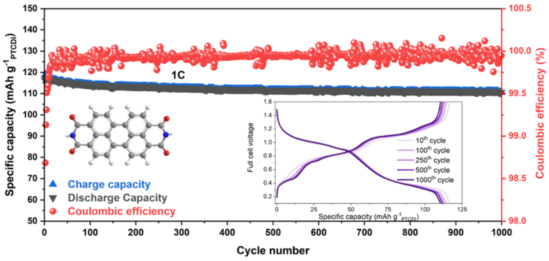

Fig 1. Long term galvanostatic cycling of an all-organic PTCDI electrode in a PTCDI/low conc. aqueous el./LFP cell set-up. Inset shows the chemical structure of PTCDI and the corresponding charge/discharge voltage curves.

ABSTRACT PROPOSAL

Lithium-ion battery electrode materials based on redox-active Covalent Organic Frameworks

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Keywords: *Redox-active Covalent Organic Frameworks, Lithium-ion batteries.*

ABSTRACT (200 words max.)

The energy sector is nowadays the main contributor towards global warming, raising the urgency for a faster transition to cleaner energy sources and consequently increasing the need for better, safer, and more sustainable energy storage solutions. This communication focuses on the use of Covalent Organic Frameworks (COFs), a type of crystalline porous polymer based on organic building blocks linked by covalent bonds, as electrode materials for lithium-ion batteries. First, the focus is centred on the synthesis and characterization of two different redox-active COFs: DAAQ-TFP-COF and TTF-BT-COF. Afterwards, the synthesized materials were used as cathodes in coin-cell type lithium batteries that were further characterized. In addition, the electrodes based on DAAQ-TFP-COF were further studied using Scanning Kelvin Probe (SKP), a non-destructive and non-invasive technique that allows the study of the chemical surface's potential on a delimited sample area. Lastly, Soft X-ray Transmission Microscopy (TXM) measurements performed at ALBA's MISTRAL synchrotron beamline were used to study the homogeneity of the state of charge within the DAAQ-TFP-COF electrodes as well as the lithiation process by using electrodes at a different state of charge and discharge and with different particle thickness. These results were useful to further uncover relations between covalent organic frameworks and their application as electrode materials for rechargeable batteries.

ABSTRACT PROPOSAL

Cationic Viologen Polymers in Anion Rocking-Chair Batteries and Full-Organic Cells

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Keywords: *Poly(vinylbenzyl)viologen, Anion Rocking-Chair Battery, Poly(3-vinyl-N-methylphenothiazine), Full-Organic Cell*

ABSTRACT

Viologens are a family of well-studied cationic redox active organic molecules with a wide use in chemistry and material science in a variety of applications, such as sensors, redox catalysts and electrochromic materials.[1] With two reversible reductions at 2.16 and 1.73 V *vs.* Li/Li$^+$, an increasing number of viologen derivatives have been developed to be deployed as active materials in organic redox flow batteries[2] as well as in solid batteries.[3,4] The immobilisation of these redox active moieties in a polymeric structure enables the fabrication of electrodes that can be utilized in anion rocking-chair batteries.

We herein present the synthesis of linear and crosslinked cationic poly(vinylbenzyl)viologens (PVBV and X-PVBV) and the investigation of their electrochemical performance. With the two reversible 1 electron redox processes, theoretical specific capacities of up to 92.7 mAhg^{-1} are achievable (considering the mass of two PF$_6^-$-anions per viologen subunit). In addition to the performance of the viologen polymers in half cells *vs.* Li/Li$^+$, X-PVBV is examined in full-organic cells as negative electrode material opposing a positive electrode containing the crosslinked poly(3-vinyl-*N*-methylphenothiazine) (X-PVMPT)[5], showing promising results.

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Discovery of degradation mechanisms of organic redox flow battery(RFB) electrolytes

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Keywords: organic redox flow battery, degradation mechanism, computational framework

Abstract: Organic redox flow batteries (RFBs) show great potential for large-scale energy storage, but their thermodynamic chemical instability is a major roadblock. The degradation mechanisms, or even final products, may not be known for new electrolytes, preventing effective mitigation strategies. This project proposes an entirely different paradigm for designing RFB electrolytes by abandoning the thermodynamic stability requirement and assuring instead that they remain kinetically stable. It will be achieved by developing a computational framework for the automated discovery of degradation reaction mechanisms and applying it to develop new kinetically stable electrolytes with optimized electrochemical properties. If successful, our approach will break new ground in sustainable grid-scale energy storage solutions.

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ABSTRACT PROPOSAL

ORGANIC FARADAIC DEIONIZATION CELL BASED ON POLYIMIDE SYMMETRIC ELECTRODES

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Keywords: *Faradaic deionization; Deionization; Polyimide; All-polymer; Rocking-chair system.*

ABSTRACT (200 words max.)

The depletion of natural freshwater sources drives the need for replacing aging-related infrastructures by new water treatment technologies. Among them, faradaic deionization (FDI) is an emerging and promising electrochemical technique to effectively address this issue. Research in this context has primarily focused on inorganic intercalation compounds typically used in batteries for energy storage [1]. However, stability issues that affect long-term performance along with safety and sustainability aspects might limit their practical deployment.

As an alternative, we introduce in this work for the first time an all-polymer FDI cell operating in a rocking-chair mechanism with the aim of boosting the deionization performance [2]. A proof-of-concept FDI cell was constructed and fully tested using the oxidized and reduced forms of redox-active naphthalene-polyimide in the respective electrodes. Our all-polymer FDI cell demonstrated a remarkable desalination capacity (155.4 mg g^{-1}) together with a high salt-removal rate (3.42 mg g^{-1} min^{-1}). In addition, long-term stability tests provided salt adsorption capacity retention values over 95 % after 100 cycles. Compared to the state-of-the-art deionization materials, the reported technique exhibits superior performance, thus making it a viable alternative for robust and sustainable "water-energy" electrochemical applications.

Acknowledgments: This project is founded by the project SELECTVALUE (2020-T1/AMB-19799) of the Talento´s program from the Community of Madrid.

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One-step non-sacrificial electrodeposition of an electrically conducting MOF on various functional substrates and microdevice integration

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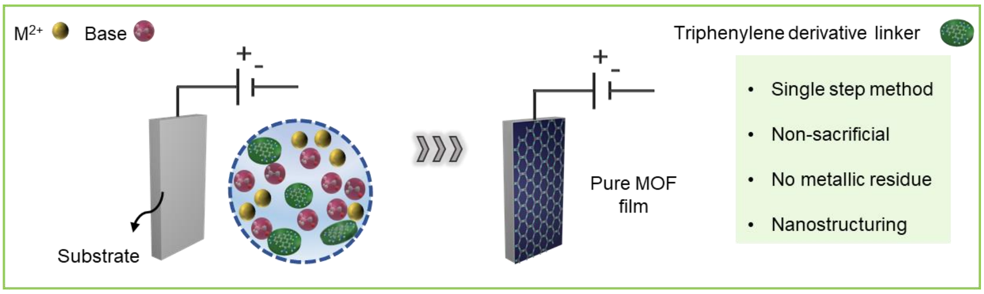
Keywords: *electrodeposition, metal-organic frameworks, nano-structuring, supercapacitors.*

ABSTRACT

The simultaneous advantages of high surface area and electrical conductivity up to 150 S.cm^{-1} have made 2D MOFs as extraordinary candidates for electrode materials in microsupercapacitors[1]. Fabricating well-defined and large area films of 2D conductive MOFs with precise controllability of thickness, morphology, and crystallinity is of crucial importance to fully take advantage of these materials as electrode materials in electronic micro/devices. Numerous research has been dedicated to establish film fabrication methods of MOF materials such as liquid phase epitaxy, gas-liquid phase interfacial, langmuir-blodgett layer by layer deposition, chemical vapor deposition *etc*[2]. Among reported methods, electrochemical deposition (ECD) is considered as the most promising one to produce high-quality 2D MOFs for electronic devices.

Herein, we introduce the innovating strategy of non-sacrificial one-step potentiostatic anodic electrochemical deposition of Ni_3(2,3,6,7,10,11-hexaiminotriphenylene)$_2$ ($Ni_3(HITP)_2$) as a model 2D MOF system. This method enables the growth of 2D MOF films on various 2D and 3D substrates and permits the growth of 3D nanostructures (nanotube/nanowire networks). The capacitive behaviour of the as-electrodeposited $Ni_3(HITP)_2$ film was ultimately tested using interdigitated micro-supercapacitor devices.



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ABSTRACT PROPOSAL

Unlocking reversible twofold oxidation in *N*-styrylphenothiazine-based polymers

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Keywords: *lithium-organic battery, p-type redox-active group, phenothiazine, polymer composite electrodes, twofold single electron oxidation, microwave chemistry*

ABSTRACT (200 words max.)

In recent years, phenothiazine (PT) has been established as a versatile building block for redox-active organic small molecules and polymers alike to be used as electrode materials for charge storage. This is mainly due to the excellent stability and reversibility of its first oxidation to form the respective radical cation. These factors result in outstanding cyclability of PT-based redox polymers at high potentials of above 3.5 V *vs.* Li/Li^+.[1-4] Unfortunately however, the second oxidation towards the dication of PT can only be achieved at voltages beyond the stability window of common electrolytes (> 4.2 V *vs.* Li/Li^+), which presents a crucial limiting factor to the capacity.We herein present a novel synthetic pathway towards a polymer-bound, donor substituted PT, effectively lowering the potential of the second oxidation step into an electrochemically exploitable range. A microwave assisted dimethoxylation of PT is the key step in the preparation of the cross-linked poly(*N*-styryl-dimethoxy-PT) (X-PDMPT), which circumvents a *de novo* synthesis of the PT core.

X-PDMPT boasts two separate one-electron oxidations at potentials of 3.38 and 3.96 V *vs.* Li/Li^+. Both processes are electrochemically reversible and stable, unlocking a high theoretical specific capacity of 143 mAh g^{-1}, and thus rendering X-PDMPT a promising candidate for various p-type energy storage applications.

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ABSTRACT PROPOSAL

Novel binders enabling Si-rich anodes for the next generation Li-ion batteries

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Keywords: *Lithium-ion batteries, Silicon anode, Binder*

ABSTRACT:

Silicon is a promising alternative anode for Li-ion batteries owing to its 10-fold larger capacity compared to conventional graphite. However, due to huge volumetric changes during charge and discharge, the silicon active material particles disintegrate and lose electrical connection with the current collector. Furthermore, the large volume changes prompt continuous solid electrolyte interphase formation, that results in low initial coulombic efficiency and severe capacity fade upon cycling.

An intense research effort is dedicated to the development of viable silicon-rich anodes, either through carbon-silicon composite preparation, silicon particles nanostructuring, optimization of the electrolyte composition, or development of specific functional binders.

This study aims at enhancing the performance of silicon-based anodes by developing novel polymer binders. The obtained binders allow for a strong interaction with silicon particles and improved ionic and electronic conductivity, resulting thus in enhanced electrochemical performance.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement N°945357

Indolocarbazole-Based Small-Molecules as p-Type Cathode Materials with Double Redox for Lithium-Organic Batteries

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Keywords: *organic rechargeable batteries, p-type, composite electrodes, indolocarbazoles, flexible batteries*

ABSTRACT (200 words max.)

Redox-active organic materials (ROMs) are drawing much attention as promising candidates for alternative electrodes owing to natural abundance and versatility. To date, most of organic electrode research, however, have employed n-type ROMs, whose redox potentials are limited below 3.0 V vs. Li/$^{+}$Li due to their redox mechanism relying on reduction. In contrast, p-type ROMs relying on oxidation mechanism accompayning anion insertion exhibit high voltage with fast rate-capability. Nevertheless, the narrow electrochemical window of typical electrolytes limits their specific capacity. In this work, we present 5,11-diethyl-5,11-dihydroindolo[3,2-b]carbazole (DEICZ) and their derivatives as new p-type ROMs for cathode materials in lithium-organic batteries. Notably, DEICZ derivatives show double redox at high voltages of 3.44/4.09 V *vs.* Li^{+}/Li within the stable electrolyte window, leading to high theoretical capacity. To improve the cycle stability and rate capability, single-walled carbon nanotubes (SWNTs) are intermixed with DEICZ, resulting in 70.4% capacity retention of the DEICZ/SWNT composite electrode after 300 cycles. Moreover, its electrochemical performance are maintained even after 1000 times of bending test. Finally, we investigate the electrochemical properties of various DEICZ derivatives to establish structure-property relationships.

ABSTRACT PROPOSAL

Electrochemical investigation of a phenothiazine polymer as positive electrode material for aluminium batteries

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Keywords: *Phenothiazine-based polymer, p-type material, aluminium organic battery*

The lithium-ion battery is the most mature energy storage technology and currently the preferred power source for portable devices. Due to the high cost and limited supply of lithium, the use of Li-ion batteries for large-scale applications is currently under discussion. Other metal anode materials such as sodium, potassium, calcium, magnesium, and aluminium, which are more abundant than lithium, have been proposed as suitable candidates for energy storage applications. Therefore, these materials are expected to reduce the cost of alternative electrochemical storage systems and provide long-term sustainability.[1,2]

Most of the commonly used cathode materials in lithium-ion batteries consist of metal oxides which are not suited for multivalent ion batteries. Intercalation and deintercalation of complex multivalent ions in inorganic materials is challenging and often results in slow kinetics and short lifetimes. The use of organic materials is an attractive alternative in this regard. The wide range of options for designing organic compounds allows for a vast variety of intrinsic structural, mechanical, and electrochemical properties.[3]

We herein present the electrochemical investigations of a phenothiazine-based polymer as positive electrode material for application in aluminium batteries. Cross-linked poly(3-vinyl-*N*-methylphenothiazine)-based electrodes deliver experimental capacities up to 167 mAh g^{-1} and exhibit high cycling stability of 5000 cycles at 10 C rate with 88 % of capacity retention.

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ABSTRACT PROPOSAL

Lithium-Phenolate (Metal-)Organic Cathodes

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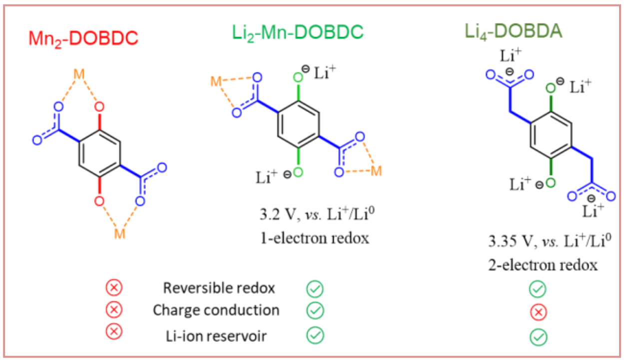
Keywords: *Organic cathodes, Metal-Organic-Frameworks, Li-reservoir*

ABSTRACT

Organic materials/Metal–organic frameworks (OMs/MOFs) have emerged as an important, yet highly challenging class of electrochemical energy storage materials. The chemical principles for electroactive OMs/MOFs remain, however, poorly explored because precise chemical and structural control is mandatory. Herein, two different Li-phenolate OMs/MOFs were disclosed with aim of raising the operating potential and enable the charge conduction. First one is electrically conducting Li-ion MOF cathodes with the generic formula Li_2-M-DOBDC (wherein M = Mg^{2+} or Mn^{2+}; $DOBDC^{4-}$ = 2,5-dioxido-1,4-benzenedicarboxylate), by rational control of the ligand to transition metal stoichiometry and secondary building unit (SBU) topology in the archetypal CPO-27 (Mn_2-DOBDC). These Li_2-M-DOBDC materials validate the concept of reversible redox activity and electronic conductivity in MOFs by accommodating the ligand's noncoordinating redox center through composition and SBU design. Secondly, although many efforts have been directed on tuning through substituent electronic effect, the chemistries than can operate above 3 V vs Li^+/Li^0, and thus be air stable in the Li-reservoir form remain finger-counted. We reveal an innovative organic Li-ion cathode material—the tetralithium 2,5-dihydroxy-1,4-benzenediacetate (Li_4-DOBDA)—with a remarkably high redox potential of 3.35 V vs Li^+/Li^0 attained notably in the solid phase.



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ABSTRACT PROPOSAL

Visible-Light Augmented Lithium Storage Capacity in a Ruthenium (II) Photosensitizer Conjugated with a Dione Catechol Redox Couple

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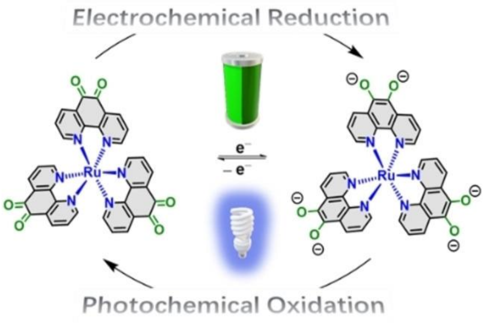
Keywords: *electron transfer; energy storage; photo-batteries; photo-induced; photosynthesis*

ABSTRACT (200 words max.)

Controlling redox activity of judiciously appended redox units on a photo-sensitive molecular core is an effective strategy for visible light energy harvesting and storage. The first example of a photosensitizer - electron donor coordination compound in which the photoinduced electron transfer step is used for light to electrical energy conversion and storage is reported. A photo-responsive Ru-diimine module conjugated with redox-active catechol groups in [Ru(II)(phenanthroline-5,6-diolate)3]4- photosensitizer can mediate photoinduced catechol to dione oxidation in the presence of a sacrificial electron acceptor or at the surface of an electrode. Under potentiostatic condition, visible light triggered current density enhancement confirmed the light harvesting ability of this photosensitizer. Upon implementation in galvanostatic charge-discharge of a Li battery configuration, the storage capacity was found to be increased by 100 %, under 470 nm illumination with output power of 4.0 mW/cm-2. This proof-of-concept molecular system marks an important milestone towards a new generation of molecular photo-rechargeable materials.



Reference: D. Gupta et al., *Chemistry–A European Journal*, **2022**, *28* (42), 202201220.

ABSTRACT PROPOSAL

Molecular Engineering of Metalloporphyrins for High-Performance Energy Storage: Central Metal Matters

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Keywords: *metalloporphyrin, multielectron redox reaction, structure-performance relationship, porphyrin metal centers, organic electrodes*

ABSTRACT (200 words max.)

The enormous number of porphyrin-based derivatives represent a new class of redox-active materials in lithium- and post-lithium systems for sustainable electrochemical energy storage. The relationship between structure and performance is poorly understood which confines the rational design of such electrode materials and subsequent access to their full potential. We systematically designed and investigate the structural and electrochemical characteristics of selected porphyrin derivatives of varying central metals to gain the understanding of the processes taking place. First-row transition metal complexes from Co to Zn of 5,15-bis(ethynyl)-10,20-diphenylporphyrin are used as models to investigate the relationships between structure and electrochemical performance. The practical voltage window and discharge capacity turned out to be strongly influenced by the metal center. Computational calculations showed that the choice of central metal atom influence the planarity of the porphyrin. The intramolecular rearrangement and packing of metalloporphyrins can be illustrated with single crystal diffraction. In addition to the direct effect of the metal choice on the undesired solubility, efficient packing and crystallinity are found to dictate the rate capability and the ion diffusion with the porosity. These findings open up a wide field of compositions and morphologies to accelerate the practical application of resource-efficient cathode materials and meet the rapidly growing demand for efficient electrical energy storage.

ABSTRACT PROPOSAL

Quinone-based Cathodes in Magnesium and Calcium based Batteries using non-corrosive [B(hfip)$_4$]-Electrolytes

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Keywords: *quinone-based Cathodes, Magnesium-/Calcium-Electrolytes*

ABSTRACT (200 words max.)

The growing demand for high-energy storage systems has led to intensive research into sustainable and low-cost battery technologies. In this context rechargeable magnesium and calcium based batteries are considered as promising candidates due to the advantages of abundant raw material resources, high theoretical energy densities and the potential applicability of metal anodes.[1] However, to develop efficient electrolytes and to find suitable cathode materials have been the key challenges. Our group have developed the non-corrosive [B(hfip)$_4$]-based electrolytes (hfip = OCH(CF$_3$)$_2$), which fulfil the requirements as practical electrolytes for magnesium and calcium battery systems.[2] Furthermore, a quinone-based polymer was proven to be suitable cathode material in both systems showing promising performances.[3] Currently, we are focusing on improving material synthesis and cathode preparation, with the aim to assembly pouch cell stacks to go from lab cell level to battery with higher TRL. Herein, we will show a summary of our investigations and results.

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ABSTRACT PROPOSAL

Organic redox polymers for multivalent ion batteries

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Keywords: *aluminium-ion battery 1, organic redox polymer 2, renewable energy 3*

ABSTRACT (200 words max.)

The global demand for renewable energies is rising. therefore, considerable studies have been devoted to developing high capacity, long cyclic life, economical, and safe batteries based on renewable and abundant active materials. To date, lithium-ion batteries are one of the most mature and efficient energy storage systems. [1] However, finding alternatives, due to the limited resources of lithium and transition metals, is crucial. Lately, organic batteries utilizing redox polymers have become promising candidates for next generation energy storage because of their facile synthesis from easily accessible resources, and their tuneable structures. Moreover, polymer incorporation can inhibit dissolution of the organic active materials in electrolytes. [2] To date, many investigations have been applied to advance organic redox polymers for charge storage. One of these is to take advantage of multivalent elements including, zinc, magnesium, calcium and aluminium due to their high theoretical energy densities, low-cost along with the high abundancy in the Earth's crust. [3] Among these, Al-ion batteries are attracting increasing attention due to the high specific capacity of Al and the non-flammability of the electrolytes. These properties enable Al-ion to stand out for large-scale electrochemical energy storage. [4] We herein present Al-based batteries using organic redox polymers as positive electrode materials.

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ABSTRACT PROPOSAL

Enhancing the Charge Storage Capabilities in Carboxylate-based Materials by Thiadiazole Fusion

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Keywords: *organic electrode material, metal-ion organic battery, carboxylates, small molecules, n-type material, …*

ABSTRACT (200 words max.)

Dicarboxylate moieties are particularly attractive in the development of metal-ion organic batteries as they can reversibility store alkali metal ions (Li, Na or K) at low working potential, while exhibiting good stability in liquid electrolytes. Although many molecular designs have been investigated in the last decade, conjugated dicarboxylates are impeded by low Coulombic efficiencies, especially at the first cycle, and sluggish kinetics in most cases.

A new strategy in the design of conjugated carboxylates is presented by fusing a thiadiazole heterocycle to a terephthalate core. We herein report the synthesis and electrochemical performance of dilithium-2,1,3-benzothiadiazole-4,7-dicarboxylate (Li_2-DCBTZ) as positive electrode material. The presence of the thiadiazole ring enables (i) a better conjugation of π-n electrons leading to a benefit in terms of rate capability, and (ii) a better stabilizing coordination network for Li ions through both oxygen and nitrogen atoms. Additionally, the reduced state Li_4-DCBTZ is stabilized due to a maintained aromaticity in the heteroaromatic core, which creates an advantage over terephthalate-based material.[1] These effects result in an average operation potential of 1.85 V *vs.* Li^+/Li and a capacity of up to 190 mAh g^{-1}. Theoretical calculations on the Li-ion storage mechanism and bonding character support the experimental work.[2]

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ABSTRACT PROPOSAL

Triazatruxene-based Covalent Organic Framework as Cathode Material for Organic Lithium Batteries

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Keywords: *Covalent Organic Frameworks, p-type Cathode Materials, Organic Batteries*

ABSTRACT

Covalent organic frameworks (COFs) containing redox-active groups are promising positive electrode materials for rechargeable batteries. However, the utilization of their entire redox-activity is always limited due to the poor electrical conductivity of the COFs, which also restricts the rate capability. Furthermore, most redox-active COFs have redox potentials below 2.5 V which limits the energy density of the resulting battery.[1,2] Herein, we present a triazatruxene-based COF with a high specific surface area of 1373 $m^2\ g^{-1}$ its composite with SWCNTs to obtain binder-free electrodes as free-standing films. This design enables to use this COF as a p-type positive electrode materials with a high reversible discharge capacity of up to 80 mAh g^{-1} at 0.2 C rate at a high average redox potential of 3.9 V *vs.* Li/Li^+, which sets a new record in redox potential among COF-based battery electrode materials.[3] Furthermore, the azatruxene-based COF-CNT exhibited excellent rate performance (49 mAh g^{-1} at 20 C rate) and a long cycling stability with 75 % retention of specific capacity at 2 C rate after 500 cycles.

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ABSTRACT PROPOSAL

Multivalent Metal Batteries with Organic Electrode Materials

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Keywords: *multivalent metal batteries, post-lithium energy storage, polymer,*

ABSTRACT (200 words max.)

Currently lithium-ion batteries are globally used as energy storage device. However, the low earth crust abundance of lithium and its high cost call for the development of alternative technologies. For post-lithium ion storage rechargeable multivalent batteries are considered a sustainable option using aluminium, calcium or magnesium as negative electrode materials. Unfortunately, the search for compatible positive electrode materials regarding output voltage, cyclability and reversibility of the electrochemical processes faces challenges. Promising candidates are organic compounds, such as redox polymers. A major advantage lies in their structural adaptivity, allowing to change their redox properties by introducing and adjusting functional groups. Benzoquinones are a well-known redox moiety used in electrode materials for charge storage due to their reversible two-electron redox reaction and stable cycling behaviour. Therefore, it is of great interest to develop and further investigate organic polymers based on benzoquinones as electrode materials for multivalent metal batteries, and we herein present examples thereof.

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ABSTRACT PROPOSAL

NOVEL GEL POLYMER ELECTROLYTES FOR LI/PTMA CELLS

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Keywords: *dopamine, UV-polymerization, Li/PTMA*

ABSTRACT

Organic batteries attracted great attention since they were reported by Nakahara *et al.*[1] for the first time due to their advantages, such as environmental friendliness, low toxicity, high mechanical flexibilitiy, and low cost. Many efforts have been made to develop novel organic electrode materials, nevertheless, there is still a gap on electrolytes for organic batteries. Although liquid electrolytes provide high ionic conductivity, they suffer from safety issues. Solid polymer electrolytes (SPEs) are safer systems than liquid electrolytes, however, their ionic conductivity is still low. Gel polymer electrolytes (GPEs), containing polymers swollen with liquid electrolyte, offer mechanical flexibility, high ionic conductivity, and high safety at the same time. In this study, novel GPEs were prepared for Li/PTMA cells. After UV-polymerizing the mixture of methacrylate- and methacrylamide-based monomers, the films were immersed in liquid electrolyte comprising an ionic liquid and a lithium salt. Thanks to the dopamine-bearing co-monomer, the GPEs reveal a high electrolyte uptake, and accordingly, high ionic conductivities were obtained. These new GPEs were successfully utilized in Li/PTMA cells and their electrochemical performance was investigated.

References

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ABSTRACT PROPOSAL

BIODEGRADABLE AND COMPOSTABLE BATTERIES FOR PRECISION AGRICULTURE AND DECENTRALIZED ENERGY SYSTEMS

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Keywords: *Environmental consciousness, compostable batteries, paradigm change, precision agriculture*

ABSTRACT

Agriculture production is facing a sustainability challenge when meeting the rapidly increased food demand from exponential population growth and at the same time, adopting ecological preservation practices. Precision agriculture has become a compulsory practice to maximize production while reducing resources consumption, using sensors, drones and machine vision.[1] Portable batteries are still the main power source in most of these devices. However, the usual remoteness of rural agricultural areas together with the lack of proper collection routes and specialized recycling facilities, yields to conventional portable batteries being disposed of directly into the natural environment.[2]

We propose a new power source paradigm based on biodegradable and compostable batteries ecodesigned to power precision agriculture sensors.[3] The combination of bioderived organic materials and carbon-based electrodes comprising these batteries has the unique feature that its waste can nurture soil or restore natural systems. This work presents the initial battery prototype developed as a reference tool to reformulate and carry out the different sustainability assessments techniques, i.e. life cycle assessment (LCA); toxicity, compostability and soil degradation standardized procedures. The methodological framework presented herein contributes to the creation of effective technological solutions that do not just pursue innovation but genuinely care, respect and preserve the natural ecosystems.

References:

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3. http://www.bideko-project.eu/

ABSTRACT PROPOSAL

Distribution of relaxation times analysis of a hydrogel electrolyte for organic batteries

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Keywords: *hydrogel electrolyte, impedance analysis, distribution of relaxation time*

ABSTRACT (200 words max.)

Organic materials offer a freedom of design regarding synthesis, which enables water-based environmentally friendly batteries. Recently, such a system was demonstrated in an organic hybrid battery consisting of an organic cathode, a water-based hydrogel electrolyte, and a zinc anode exhibiting a high cyclability of over 30,000 cycles. Electrochemical impedance spectroscopy is a non-destructive method for the analysis of electrochemical systems, more specifically, the impedances of the underlying polarization processes. Identifying those polarization processes is crucial for understanding the whole system and its impedance spectrum. Distribution of relaxation time (DRT) analysis is a supportive method for the identification of those polarization processes and their respective time scales. DRTs have already been applied in energy storage research, but – to the best of our knowledge – not for a hydrogel electrolyte used in a battery. There is a general lack of those investigations in organic battery literature. Thus, we focus here on a DRT analysis of a hydrogel, particularly on the method itself including the accuracy of the impedance measurement and its consequent transformation into a DRT as well as their interpretation.

ABSTRACT PROPOSAL

Water soluble polymers for redox-flow batteries

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Keywords: *RFB, polymer, block copolymer, RAFT, PISA*

Redox-flow batteries (RFB) are an emerging technology in energy storage for stationary applications. Redox-active polymeric materials are developed to reduce the cost of the separator by using a simple size exclusion membrane[1]. Here we present a different array of structures for aqueous polymer RFBs. Linear water-soluble copolymers were obtained by reversible addition-fragmentation chain transfer (RAFT) with tetramethylpiperidyl-methacrylate (TPMA) as precursor for the TEMPO nitroxide-radical and methacrylamide-propyltrimethyammonium chloride (MAPTAC) as solubility mediator. The degree of polymerization (DP) of the obtained polymer ranges from 30 to 80, and with narrow dispersity (Đ~1.2). Similar polymers were also obtained using tetramethylpiperidyl-methacrylamide (TPMAm) as TEMPO precursor, a more hydrophilic moiety.

These polymers were then developed into particles via polymerization induced self-assembly (PISA) by chain extension with a hydrophobic monomer, e.g. BzMA (benzylmethacrylate). The obtained polymers and colloidal suspensions were characterized by size exclusion chromatography (SEC), dynamic light scattering (DLS), cryogenic transmission electron microscopy (cryo-TEM) and analytical ultracentrifugation (AUC).

Controlled polymerization (RAFT) and PISA were employed to obtain different water-soluble polymer structures with redox active groups and its precise characterization was possible by employing a combination of different techniques.

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ABSTRACT (200 words max.)

ABSTRACT PROPOSAL

Pentacene-5,7,12,14-tetraone based polymers as cathodes for sodium batteries

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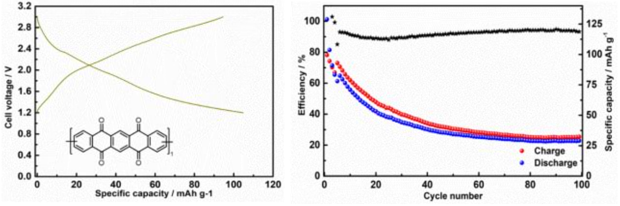
Keywords: *polymer cathode, pentacene-5,7,12,14-tetraone, sodium battery*

ABSTRACT (200 words max.)

Pentacene-5,7,12,14-tetraone (PT) is a highly effective cathode material in metal batteries with aqueous electrolytes due to its high theoretical capacity of 316 mAh.g^{-1}.[1] This capacity is achieved thanks to the presence of two quinone functional groups in the aromatic core. PT is not very soluble in aqueous medium, due to the absence of polar functional groups, making it well-suited for use in aqueous environments. By contrast, when used in non-aqueous systems with monovalent ions, PT-based electrodes suffer from rapid capacity fade, due to the dissolution of active material into the electrolyte.

One way to prevent such dissolution is through polymerization. Here, we show that dibromo-PT can be polymerized into a poly(pentacenetetraone) (PPT) by Yamamoto coupling. We use PPT as a cathode against a Na foil anode with 1 M $NaPF_6$ in EC: DMC (1:1) electrolyte. The resulting cell demonstrates an initial discharge capacity of approximately 130 mAh g^{-1} in the first cycle, and it retained 25% of that capacity at the end of 100 cycles. In the 20th cycle, the cell exhibited a coulombic efficiency of 87%, which stabilizes at 95% beyond the 50th cycle. This shows that PPT is less prone to dissolution, representing a promising new cathode material for metal batteries.



ABSTRACT PROPOSAL

Morphology-Electronic Property Relationships in Radical-Containing Polymers for All-Organic Batteries

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Keywords: *radical-containing polymers, molecular dynamics, all-organic batteries*

ABSTRACT (200 words max.)

The increasing societal need for energy storage, currently essentially relying on the lithium-ion battery technology, presents pressing challenges that include the full life cycle of the batteries, their carbon footprint, and their reliance on scarce metals. Among emerging technologies, organic-based batteries may offer metal-free solutions to energy storage. One example of such emerging battery technologies are solid-state devices that use nonconjugated radical-containing polymers as anode and cathode materials. However, a fundamental understanding of how the chemical structure of such redox-active polymers impacts their performance is still lacking, hindering progress.

Using atomistic molecular dynamics, electronic structure calculations, and machine learning, we investigate structural and electronic properties of novel phthalimide-containing redox-active polymers. We systematically investigate polymer-electrolyte systems and vary the polymer backbone chemistry, electrolyte solution content, and polymer state of charge. As a function of such system parameters, we then investigate in detail structural properties – such as phthalimide-phthalimide conformations, and the electrolyte distribution in the polymer matrix – and electronic properties – such as electronic couplings and charge transport networks. The derived morphology-electronic structure relationships inform the design of radical-containing polymers with improved characteristics for all-organic battery materials.

ABSTRACT PROPOSAL

Pillar[5]quinone as a high-capacity organic cathode with a highly concentrated electrolyte for rechargeable Na-ion batteries

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Keywords: *pillar[5]quinone, cathode, sodium-ion batteries, highly concentrated electrolyte, dissolution inhibit*

Small molecule organic electrode materials have potential applications in rechargeable sodium-ion batteries owing to their high capacity and cost-effectiveness. [1,2] However, they suffer from poor cycling stability and low Coulombic efficiency due to significant active material dissolution into the electrolyte. Herein, a highly concentrated electrolyte (HCE) is utilized in a carbon-encapsulated pillar[5]quinone (P[5]Q) positive electrode achieving improved capacity and cyclability. The highly viscous HCE lacks free solvent molecules and, thus, suppresses the dissolution of P[5]Q in the electrolyte and furnishes excellent electrochemical performance. Remarkably, in 5 M sodium bis(fluorosulfonyl)amide dissolved in succinonitrile electrolyte, the P[5]Q electrode displays an initial capacity of 434 mAh g^{-1} (C_{theo} = 446 mAh g^{-1}) and maintains 60% of this capacity and a high Coulombic efficiency (~98%) at the end of 120 cycles at a current rate of 0.2 C. Furthermore, the as-assembled sodium-ion battery shows excellent rate capability and prolonged cycling stability with a capacity higher than 150 mAh g^{-1} over 750 cycles at 1 C. The carbon-encapsulated P[5]Q cathode integrated with the HCE demonstrates one of the best electrochemical performances for P[5]Q in Na-ion batteries.

Reference

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ABSTRACT PROPOSAL

Modelling the Li-ion insertion in organic electrode materials: energy minimum vs. metastable phases

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Keywords: *organic electrode materials, atomic scale modelling, Li-ion insertion, metastable phases, evolutionary algorithm*

ABSTRACT (200 words max.)

The organic electrode materials (OEM) are emerging as a promising alternative to develop greener and sustainable battery technologies. However, significant improvements are still required in their cycling stability, rate capability and energy density in order to become a competitive alternative. This can only be achieved through a fundamental understanding of the electrochemistry at molecular level establishing the structure-properties relationships. To contribute to this end, we developed methodologies based on evolutionary algorithms (EA) [1,2] and potential-mapping algorithms (MAP) [3] to resolve the crystal structure of the different lithiated phases. These methods unveil different lithiation pathways, which help exploring the formation of metastable phases and one or multi-electron reactions, which constitute phenomena that are still poorly understood for organic intercalation electrodes. When comparing to experimental outcomes, it is demonstrated that metastable phases with specific molecular features are more likely to be controlling the redox reactions thermodynamics, and consequently the battery voltage. The MAP showed to be a promising methodology to assess the metastable phases during Metal-ion insertion in organic based electrodes.

[1] C. Marchiori et al., J. Phys. Chem. C 2019, 123, 4691−4700
[2] R. P. Carvalho et al., Mater. Adv., 2021,2, 1024-1034
[3] R. P. Carvalho et al., ChemSusChem 2022, e202200354

ABSTRACT PROPOSAL

FAIR data-empowered active learning for the accelerated discovery of redox-active polymers for metal-free batteries

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Keywords: *Redox-active polymers, FAIR data, energy storage, active learning, molecular dynamics, density functional theory*

ABSTRACT (200 words max.)

Polymer informatics has great potential to accelerate materials development for diverse applications including solar cells and energy storage. However, adoption of big-data methods to polymers has been slow, largely due to the lack of data reported in a machine-readable format, discouraging community reuse. To address this issue, polymer-specific, machine-readable data must be curated with high findability, accessibility, interoperability, and reusability (FAIRness). One class of polymers that stands to benefit are redox-active polymers (RAPs), which consist of a non-conjugated backbone and side-groups that contain stable radicals, key to their electrochemical functionality and promise as battery materials. While RAPs have an extensive chemical design space due to the vast number of possible side-groups, optimizing this space presents a significant challenge. Thus, highly descriptive yet organized data is required for the targeted design of RAPs. In this project, multiscale simulation methods including density functional theory and atomistic, coarse-grained, and ab initio molecular dynamics are utilized to evaluate RAP electrochemical properties. Combined with a FAIR data storage platform called the Community Resource for Innovation in Polymer Technology (CRIPT), active learning models can propose novel high-performing RAP electrode materials as new information as it becomes available, allowing efficient and high-throughput sampling of the chemical space.

ABSTRACT PROPOSAL

Disentangling the charge storage mechanism of quinone-based organic electrode materials in aqueous electrolytes

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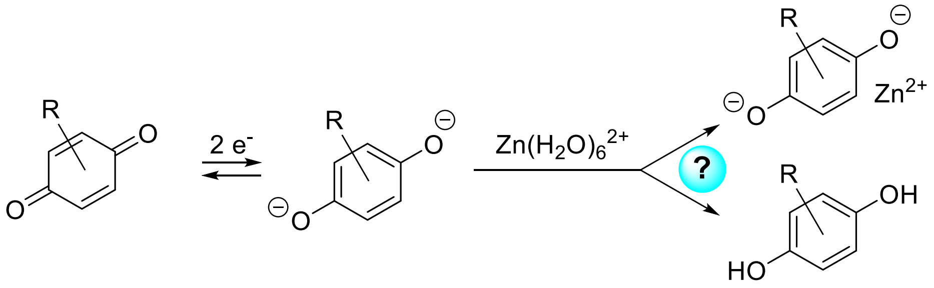
Keywords: *Aqueous electrolyte, metal-organic battery, charge storage mechanism, quinone*

The very large-scale development of rechargeable battery systems capable of storing electricity produced by renewable energies is an important issue in the energy transition. These batteries will have to meet demanding cost, durability, safety and environmental criteria.

This currently motivates a strong resurgence of interest in rechargeable aqueous batteries, in particular hybrid batteries combining, for instance, a positive electrode based on a redox-active organic material such as a quinone with a metallic electrode such as zinc. However, a major problem facing the development of these aqueous rechargeable hybrid batteries is the lack of consensus on charge storage mechanisms, which is problematic for concrete applications.

This prompted us to study in detail the electrochemical behavior of an organic electrode based on two different substituted 1,4-benzoquinones, namely *p*-chloranil and duroquinone, in the presence of buffered and unbuffered electrolytes with different pH and compositions. The results of our study have allowed us to propose a comprehensive model of the charge storage mechanism and to clearly identify the nature of the charge carrier. As a result, we gained a better understanding of the problems associated with capacity loss, potential shift, precipitation and dissolution reactions in these systems.



ABSTRACT PROPOSAL

Tailored battery electrolytes for redox-active organic molecules

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Keywords: *Organic electrode, Small molecules, Liquid electrolytes, Solvent-solvent and solvent-salt ratio*

ABSTRACT

Small redox-active organic molecules promise high specific capacities, but their high solubility poses a great challenge towards their use in rechargeable batteries. Increasing the salt concentration in the electrolyte has been reported as a suitable strategy to address this issue, but might negatively impact the ionic conductivity and, in particular, the cost of the battery.

Herein, we present a new redox-active molecule for lithium batteries with long-term stable cycling, enabled by the careful design of the electrolyte composition. We found that the electrochemical performance of the small molecules, specifically the reversibility of the redox process and its kinetics, is highly dependent on the electrolyte used, i.e., the choice of the solvent(s), lithium salt(s), and the solvent-solvent and solvent-salt ratio. As a result, the electrodes based on such small molecule provides substantially enhanced cycling stability and rate capability when using a tailored electrolyte. Following these results, we performed an in-depth *ex situ* investigation *via* various complementary techniques to gain a comprehensive understanding of the underlying principles.

A step towards Sustainability – Aqueous Processing of Organic Redox Polymers for Next-Generation Organic Batteries

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Keywords: *PVMPT, Redox polymer, Aqueous processing.*

ABSTRACT

Poly (3-vinyl-N-methylphenothiazine) PVMPT, a p-type material, is of particular interest due to its excellent rate capability, cyclic stability, reasonable theoretical capacity (112 mAh g^{-1}), and reversible redox activity. However, the electrode processing of PVMPT involves the use of conventional PVDF binder and NMP as a solvent, negating the unique properties of non-toxicity, sustainability, and safety of organic materials. Herein, we demonstrate the electrochemical performance of PVMPT with aqueous binders, such as carboxymethyl cellulose (CMC), sodium alginate (SA), and styrene-butadiene rubber (SBR). Among all, the CMC:SBR (7:3 %wt.) composition showed comparable performance to PVDF-based binders. At 1C, CMC+SBR binders delivered the initial discharge capacity of 92 mAh g^{-1} for 500 cycles, which is very close to the PVDF/NMP binders, that delivered the initial discharge capacity of 100 mAh g^{-1} for 500 cycles. The possible reason for the improved performance of PVMPT in CMC:SBR (7:3 %wt.) systems over other aqueous binders might be due to the proper dispersion of the material and enhanced adhesion of SBR to the current collector which will be further discussed in detail. Hereby, we believe the use of aqueous binders will enable us to achieve sustainability by providing eco-friendly and 'green' energy storage systems.

ABSTRACT PROPOSAL

Revealing the Reversible Solid-State Electrochemistry of Lithium-Containing Conjugated Oximates: Towards a New Functionality for Organic Batteries

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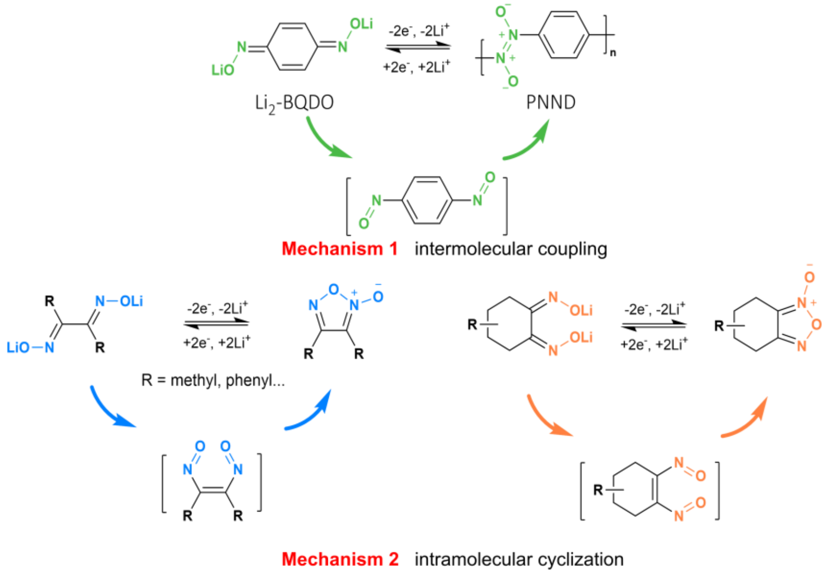
Keywords: *conjugated oximates, functionality, Organic batteries*

In the rising advent of organic Li-ion positive electrode materials with increased energy content, chemistries with high redox potential and intrinsic oxidation stability remain a challenge. Herein, we report the solid-phase reversible electrochemistry of the oximate organic redox functionality. The disclosed oximate chemistries, including cyclic, acyclic, aliphatic and tetra-functional stereotypes, uncover the complex interplay between the molecular structure and the electroactivity. Amongst the exotic features, the most appealing one is the reversible electrochemical polymerization accompanying the charge storage process in solid phase, through intermolecular azodioxy bond coupling. The best performing oximate delivers a high reversible capacity of 350 mAh g^{-1} at an average potential of 3.0 vs. Li^+/Li^0, attaining 1 kWh kg^{-1} specific energy content at the material level metric. This work ascertains a strong link between electrochemistry, organic chemistry, and battery science by emphasizing on how different phases, mechanisms and performances can be accessed using a single chemical functionality.



Reference: Sci. Adv., 2023, eadg6079

ABSTRACT PROPOSAL

Understanding the Ionic Conduction in Solid Polycarbonate-Garnet Composite Electrolytes

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Keywords: *Solid composite electrolyte, Ionic transport, Polycarbonate PTMC, Garnet LLZO*

ABSTRACT (200 words max.)

Solid electrolytes are considered as a key component in all-solid-state batteries. Understanding the ionic transport mechanism is crucial towards their implementation in commercial ASSBs. While PEO-based composite electrolytes have been widely studied, alternative polymer matrices have been poorly explored. In this work, we focus on investigating the Li-ion transport in a composite system containing poly(trimethylene carbonate) (PTMC) with LiTFSI as polymer matrix, with a garnet-type $Li_{6.7}Al_{0.3}La_3Zr_2O_{12}$ (LLZO) ceramic filler. This work provides insights over a fully-comprehensive electrolyte platform from lower to higher ceramic content. We show that the ionic conduction in PTMC: LLZO composite electrolytes is dependent on the particle loading. Incorporating a low ceramic loading can contribute to increase the ionic conductivity via a formation of an additional transport pathway along the polymer-ceramic interfaces. However, higher ceramic loadings have a detrimental effect on the conductivity, explained by particles agglomeration and higher resistivity of interfaces. This study shows that the ceramic concentration along with surface chemistry of LLZO has a direct effect on the Li^+-ion conduction mechanism occurring in PTMC:LLZO composite electrolytes.

Organic Battery Days 2023

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