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ElectROBatt CONFERENCE

Electrochemistry of Batteries and Energy Storage Technologies

Book of Abstracts

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October 31st to November 1st 2024
Bucharest, Romania

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Electrochemistry of Batteries and Energy Storage Technologies – ElectROBatt 2024 Conference
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ELECTROBATT

Electrochemistry of Batteries and Energy Storage Technologies

ElectROBatt 2024 Conference

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Practical Information

Oral presentations

Keynote lectures are 30 minutes long (25 minutes for the presentation and 5 minutes for Q&A). Oral presentations are 15 minutes long (we recommend a 10–12-minute talk and 3-5 minutes for Q&A). All talks should be accompanied by PowerPoint or PDF presentation slides. Presenters are kindly invited to bring their presentations on October 30, starting at 14:00, or during the break before their scheduled presentation to the person responsible for transferring them to the conference computer. We kindly ask all participants to adhere closely to the allocated duration for oral presentations.

Poster presentations

Poster boards are allocated in the space adjacent to the conference room—*Prefunction area*, and materials for setting up the posters are available at the registration desk. The poster board dimensions are 70 cm (width) by 100 cm (height). The boards are fully white. Please use tape, pins are not allowed! Attendees can preview their posters on the morning before the formal presentation. Authors need to be present at their posters for discussions with attendees during the session. Please display your poster on the board assigned with the code number (refer to the Poster Presentation section in the Conference Programme). It is each author's responsibility to remove their poster immediately at the end of the session on November 1, 2024. ElectROBatt assumes no responsibility for posters left up after this time.

Greetings of the organizers

Another brick for a sustainable energy future …

The inaugural ElectROBatt 2024 is set to be a premier gathering dedicated to the advancement of battery technologies and energy storage solutions. Organized by the National Research and Development Institute for Cryogenic and Isotopic Technologies (ICSI Rm. Vâlcea) in collaboration with Université catholique de Louvain (UCLouvain), this edition will take place in the historic city of Bucharest, Romania, from October 31 to November 1, 2024. It will bring together leading experts, researchers, and industry pioneers who are passionate about exploring the frontiers of electrochemistry.

In response to rapid technological innovation and the increasing demand for sustainable energy alternatives, ElectROBatt 2024 aims to inspire participants to delve into the latest advancements in the electrochemistry of energy storage applications. This event serves as an exceptional platform for sharing knowledge, exchanging experiences, and forging meaningful connections with peers and thought leaders from around the globe.

ElectROBatt 2024 will explore a diverse array of critical topics at the forefront of battery technologies and energy storage solutions. Key areas of focus will include advanced battery materials and chemistries, novel electrode architectures, innovative electrolyte designs, the digital edge, and smart functionalities in batteries, along with modeling and simulation approaches. This conference aims to foster discussions that address both the challenges and opportunities associated with the global demand for cleaner, more efficient energy technologies, bridging the gap between pioneering research and practical applications.

It is our pleasure to welcome you to ElectROBatt 2024, where we aim to unite a diverse community of researchers, industry leaders, and pioneers dedicated to advancing battery technologies and energy storage solutions. By supporting and empowering the next generation of battery technology, we can effectively tackle the pressing energy challenges of our time and contribute to shaping a more sustainable future.

We are confident that each of you will play an essential role in making ElectROBatt 2024 a resounding success. Let’s take full advantage of these two days dedicated to significant scientific exchange, with the goal of collecting new knowledge and fostering meaningful collaborations.

We wish you a joyful time in Bucharest and an inspiring ElectROBatt 2024 conference!

On behalf of the Organizing Committee,

Mihaela BUGA & Alexandru VLAD

ElectRoBatt 2024

Bucharest, Romania

October 31st to November 1st 2024

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Imperial College London, UK

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Fudan University, China

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ENTROPY DESIGNED ELECTRODES AND ELECTROLYTES

Patrik Johansson[1,2], Mirna Alhanash[1], Sajid Alvi[1], Carolina Cruz[1], Yihu Li[1],
Clément Pechberty[1], Johanna Timhagen[1] and Jonathan Weidow[1]

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It is a trend to talk about designed and high-entropy electrolytes (HEEs). Add to this that high-entropy alloys (HEAs) and oxides (HEOs) can be applied as negative and positive electrodes for batteries. The role of entropy is, however, not always clear – or even present. We have here created HEAs and HEEs taking care to actually outline/probe the role of entropy for the observed properties and performance.

For HEAs the main feature is that the mechanical instability caused by the large expansion and contraction associated with alloying electrodes' (de)sodiation/lithiation, and hence bad cyclability, can be mitigated by entropy design. Our proof-of-concept HEA $BiSbSe_{1.5}Te_{1.5}$ shows improved cycling stability for conversion-alloying (de)lithiation reactions; ≥20x more stable cycles than for comparable metal-Se and -Te-based anodes [1]. This comes along with a reversible capacity >450 mAh g^{-1} and without any need to use carbonaceous materials to create a composite.

Turning to HEEs we use molten salt electrolytes (MSEs) where the compositional/mixing entropy is correlated *vs.* the decreased melting points that we obtain for solvent-free equimolar MSEs [2]. We have created both mixed-cation and mixed-anion MSEs and this provides a unique mapping of entropy contributions to the stability towards (re-)crystallization, as shown by Raman spectroscopy. Furthermore, molecular dynamics simulations alongside density functional theory calculations have been used to elucidate the local structure of these MSEs, that are stepping-stones towards completely solvent-free, semi-solid, and ideally room-temperature Ca-conducting electrolytes – the grand aim.

And while not really HEEs, I will also showcase our work on deep eutectic electrolytes (DEEs) and especially how we look at molecular-level heterogeneity, as well as dual-salt electrolytes (DSEs), which are multicomponent systems where the diversity in the 1st solvation shell seems vital. The latter type of electrolytes is perhaps also the one most commonly encountered as a "HEE" in the literature.

Key words: Electrolyte, entropy, structure, dynamics, alloying, solvent-free

Acknowledgements

We acknowledge the financial support from the Swedish Research Council (grants #2020–03988 and #2021–00613) and from the Sweden's Innovation Agency VINNOVA/Battery Alliance Sweden (BASE) (grant 2019-00064) and the ALBA synchrotron for beamtime (proposal 2022097047).

References

1. Alvi, S. et al., Entropy stabilized cycling of lithium-ion battery conversion-alloying anodes, *Batteries & Supercaps*, 2024, e202300585
2. Timhagen, J. et al., Local structure and entropic stabilization of Ca-based molten salt electrolytes, *Batteries & Supercaps*, 2024, e202400297

BEYOND *Li*: *Na* AND *K* BATTERY ANODES: PROGRESS, CHALLENGES AND PERSPECTIVES

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To mitigate the climate change and reach a carbon neutral society before it is too late, a mix of sustainable energy technologies are needed.

Batteries will continue to play a vital role in decarbonising transportation as well as in storing the intermittent renewable energy. Li ion batteries have revolutionised the electrification of transportation and contributed significantly to grid storage. However, there are increasing concerns with the availability of the minerals currently used in Li-ion batteries today, especially looking at the predicted growth of batteries demand. Diversification of battery technologies with more sustainable options in mind, not only for the raw minerals used in future batteries but also for more sustainable manufacturing practices for cells and packs are needed.

In my talk I will touch on some of these sustainable practices needed to be implemented today while showing the 12 principles of “green batteries” inspired from “green chemistry” my research group introduced. I will than focus on Na-ion batteries, the next battery technology in line for commercialisation in 2024, with emphasis on our research on hard carbon anodes on understanding the fundamentals on Na ion storage using a mix of characterisation techniques coupled with electrochemistry. I will also discuss the importance and complexity of solid electrolyte interfaces and some perspectives on commercialisation from our group.

I will also resent some new insights onto a very old research topic: intercalation of alkali metals into graphite. We have performed in depth study on K intercalation in graphite using a combination of Raman (including looking at the low frequency band), XRD, dilatometry, optical microscopy as well as DFT calculation which when coupled with electrochemistry and post-mortem TOF-SIMS reveal the formation of a solid electrolyte interface responsible for capacity loss in the first cycles.

NIOBIUM PENTOXIDE AS HIGH-POWER LITHIUM-ION ANODE MATERIAL

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Lithium-ion batteries (LIBs) represent the state-of-the-art energy storage technology for powering electronic devices and are the basis for electrifying the mobility sector. However, for the latter, current LIBs need further improvement concerning their energy and power density, particularly to overcome the fast-charging limitations of the currently used graphite anode. [1, 2] Nb_2O_5 is a promising high-power anode candidate with rich structural chemistry and at least 12 polymorphs, which can be obtained based on different precursors and calcination temperatures. [3, 4] Among these polymorphs, monoclinic Nb_2O_5 (H-Nb_2O_5) provides the highest and most stable specific capacity in the voltage range from 1.0 V to 3.0 V, while orthorhombic Nb_2O_5 (T-Nb_2O_5) delivers a very stable high capacity when lowering lithiation cut-off potentials.

Herein, we present our in-depth understanding of the correlation between synthesis methods and structural evolution, as investigated through X-ray diffraction, X-ray absorption spectroscopy, and Raman spectroscopy. The electrochemical performance of different Nb2O5 polymorphs was comprehensively evaluated in both half-cells and full-cells, using high-energy $LiNi_{0.8}Mn_{0.1}Co_{0.1}$ (NMC_{811}) as the cathode material. Furthermore, the performance of these full-cells was further optimized by tuning the N/P ratios, electrolyte compositions, and introducing additional lithium sources.

Key words: lithium-ion batteries; anode materials; Nb_2O_5

Acknowledgments

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References

1. Y. Liu, Y. Zhu, Y. Cui, *Nat. Energy,* 2019, *4*, 540–550.
2. J. Asenbauer, T. Eisenmann, M. Kuenzel, A. Kazzazi, Z. Chen, D. Bresser, *Sustain. Energy Fuels,* 2020, *4*, 5387–5416.
3. X. Xue, J. Asenbauer, T. Eisenmann, G. O. Lepore, F. d'Acapito, S. Xing, J. Tübke, A. Mullaliu, Y. Li, D. Geiger, J. Biskupek, U. Kaiser, D. Steinle, A. Birrozzi, D. Bresser, *Small Struct.* 2024, 2300545
4. K. J. Griffith, A. C. Forse, J. M. Griffin, C. P. Grey, *J. Am. Chem. Soc.* 2016, *138*, 8888-8899.

POTASSIUM BATTERIES WITH LIGNIN-DERIVED HIGHLY STABLE ANODES

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In recent years, potassium ion batteries (KIBs) have drawn a lot of interest due to the increasing demand for energy, the limited availability of lithium resources, and the unique advantages of KIBs. These advantages include low cost, abundant potassium resources (2.09% of the Earth crust), a relatively low reduction potential (≈2.936 V vs. SHE), and technological similarities with established lithium-ion batteries (LIBs) [RAJAGOPALAN]. Additionally, KIBs benefit from the weaker Lewis acidity of potassium ions, leading to higher conductivity and greater quantities of solvated and transported potassium ions compared with lithium ions. Furthermore, the low desolvation energy of K+ can facilitate faster diffusion through the electrolyte/electrode interface. Despite these benefits, KIB technology is still in its developmental stage. Therefore, our research focuses on the development, study, and optimization of anode electrodes using lignin, a readily available and sustainable biomass precursor.

In this work, we synthesized two lignin-based carbon materials derived from softwood and hardwood sources to produce anodes. These biocarbon materials were activated with varying proportions of potassium hydroxide and subjected to comprehensive physicochemical characterization, including SEM, XRD, XPS, and Raman spectroscopy. Electrochemical techniques such as galvanostatic cycling, EIS, CV rate analysis, and C-rate testing were employed to assess their suitability as KIB anodes, with further optimization of electrode and electrolyte compositions. These assessments revealed that the interplanar distance and the amount of defects in the biocarbon material significantly influence the electrochemical performance of the cell. As a result, we achieved cells with favorable reversibility and capacity retention, high efficiency, and excellent long-cycle performance, utilizing a renewable source and scalable processes.

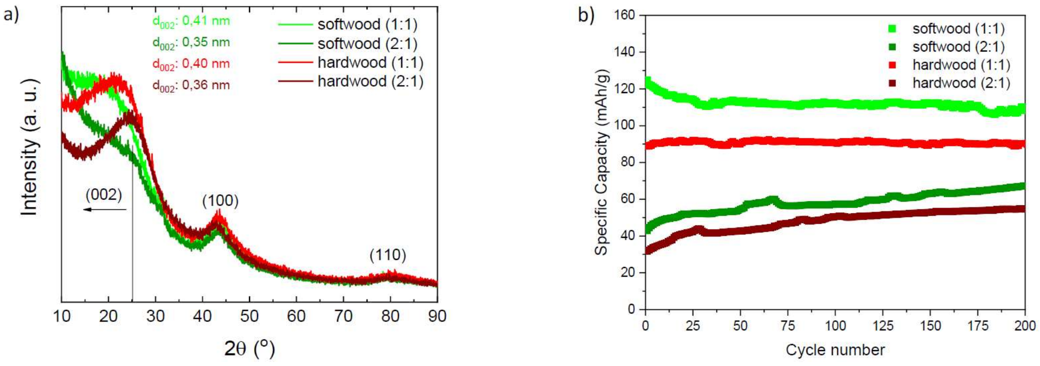

Fig. 1: *a) XRD patterns of biocarbon powder materials. b) Lignin-based anodes cycling performance (0.05 A/g).*

Key words: potassium batteries, biocarbon, lignin, anodes.

Reference

[RAJAGOPALAN], Ranjusha, et al. Advancements and challenges in potassium ion batteries: a comprehensive review. *Advanced Functional Materials*, 2020, vol. 30, no 12, p. 1909486.

HARD CARBONS FOR Na-ION BATTERIES: WHERE WE ARE AND CAN WE DO BETTER?

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Sodium ion batteries are credible alternatives to lithium ion batteries owing to the abundance of sodium, the use of non-critical materials, satisfactory performance and increased safety. Hard carbon (HC) materials are undeniably one of the most suitable anodes for sodium-ion batteries (SIBs). They can be obtained from renewable resources (Fig. 1), [Ghimbeu et al., 2024] and present high capacity, long-term cyclability, and reasonable initial Coulombic efficiency (iCE). These performances are strongly linked to the HC properties, the electrolyte type, and the electrochemical testing conditions used. In this work, several aspects will be presented including the HC synthesis, in-depth characterization of these materials, and the relationship between HC properties and performance [Beda 2021; Escamilla, 2023]. The formation of solid electrolyte interphase (SEI) and Na ion storage mechanisms (Fig.1-right), will also be discussed [Zhang 2016; Beda 2021; Ghimbeu 2024]. Nevertheless, the challenges of HC for practical utilization in Na-ion batteries will be addressed.

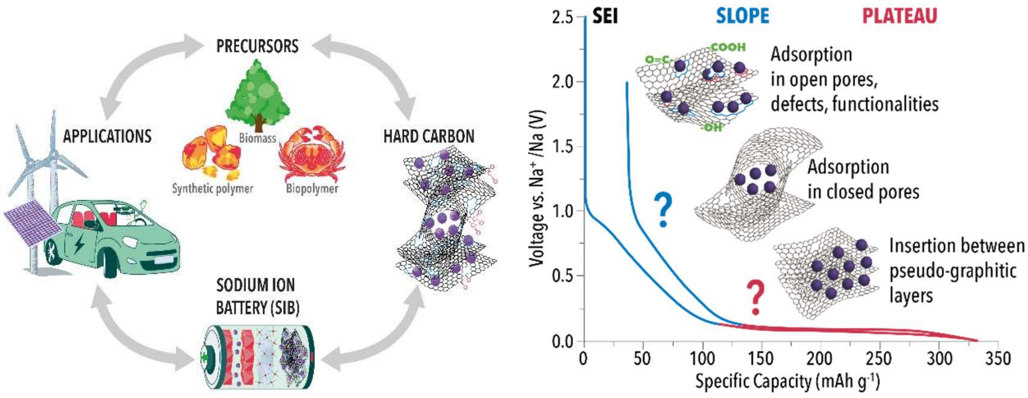

Fig. 1: *(left) Scheme showing the chain from precursor to hard carbon, Na-ion battery and potential applications. (right) Schematic representation of all possible Na-ion storage mechanisms [Ghimbeu et al., 2024].*

Key words: Hard carbon; Na-ion batteries; microstructure; storage mechanism; interface.

Acknowledgments

All students, colleagues and collaborators that contribute to this work are acknowledged, along with financial support from different agencies.

References

1. Beda A, Rabuel F, Morcrette M, Knopf S, Taberna PL, Simon P, Ghimbeu C, J Mater Chem A 9 (2021), 1743
2. Beda A, Villevieille C, Taberna PL, Simon P, Ghimbeu CM, J Mater Chem A 8 (2020), 5558
3. Escamilla AM, Beda A, Simonin L, Grapotte M, Le-Meins JM, Ghimbeu C, ACS Appl Energy Mater 6 (2023), 7419
4. Ghimbeu C, Beda A, Réty B, El Marouazi H, Vizintin A, Tratnik B, Simonin L, Michel J, Abou-Rjeily J, Dominko R, Adv Energy Mater 14 (2024) 2303833
5. Zhang B, Ghimbeu CM, Laberty C, Vix-Guterl C, Tarascon JM, Adv Energy Mater 6 (2016), 1501588.

ENGINEERED NANO-POROSITY IN SILICON-DOMINANT ANODES FOR HIGH ENERGY DENSITY AND LOW VOLUME EXPANSION

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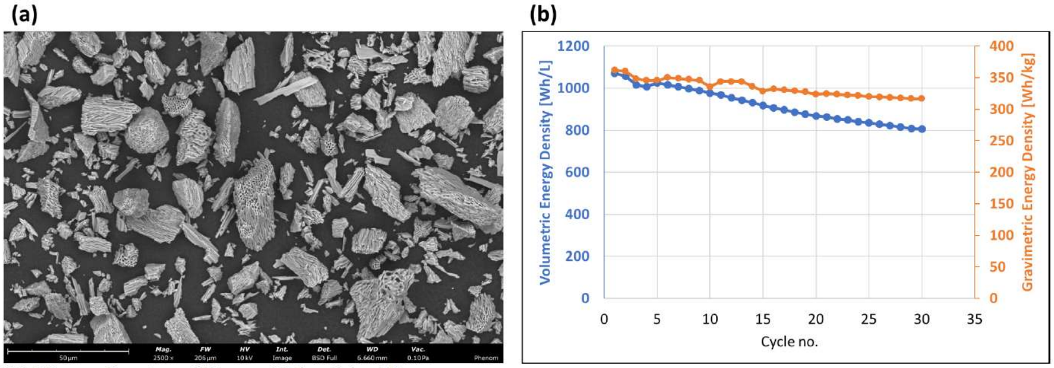
The current generation of lithium-ion batteries (LIBs) relies on graphite anodes [1]. Introducing silicon (Si) into the anode can enhance both the volumetric and gravimetric energy density [2], which is necessary to meet the demands of more advanced applications (e.g., automotive, drones, consumer electronics). However, Si-dominant anodes encounter challenges due to volume expansion during lithiation, leading to particle pulverization and safety concerns [3]. In this context, a novel micrometersized nano-porous Si material is presented, offering improved buffering of volume expansion and enhanced cell performance [4].

E-magy's silicon material is produced through a rapid directional solidification process, which allows precise control of its nano-porosity. Si-dominant slurries were prepared using Polyacrylic Acid (PAA) binder, KS6 graphite, and single-walled carbon nanotubes (SWCNTs), and then cast on a 10.3µm Cu current collector with an areal mass loading in the range of 2.84-3.19mg.cm^{-2}. CR2032 coin cells were tested with 1M $LiPF_6$ in an EC:EMC + FEC electrolyte and subjected to galvanostatic charge/discharge cycling within a voltage window of 2.8-4.3V.

Morphological characterization using SEM microscopy revealed that the Si material consists of micrometer-sized porous particles, with BET measurements indicating a specific surface area of 5m^2.g^{-1} and pore diameters ranging 200-400 nm. The electrochemical results demonstrated the feasibility of Si cycling at high specific capacity, showing gravimetric and volumetric energy densities exceeding 360 Wh/kg and 1060 Wh/L at the unit-cell stack level, respectively. These results underscore the importance of precisely tuning the particle morphology of micrometer-sized Si to maximize energy efficiency while maintaining cost-effectiveness.



SEM Image Courtesy of Thermo Fisher Scientific

Fig. 1: *(a) SEM image of E-magy's micro-particles (b) Energy density profiles (volumetric and gravimetric) of E-magy's Si-based anode (>80%) coupled with a high-nickel cathode.*

References

1. M. Armand et al., *J. Power Sources*, 479, 228708 (2020).
2. M. Marinaro, D. Bresser, E. Beyer, P. Faguy, K. Hosoi, H. Li, J. Sakovica,K. Amine, M. Wohlfahrt-Mehrens, and S. Passerini, *J. Power Sources*, 459, 228073 (2020).
3. M. N. Obrovac, *Current Opinion in Electrochemistry*, 9, 8 (2018).
4. F. Maroni et al. *J. Electrochem. Soc*. 169 08050 (2022).

UPSCALING OF TIN-CARBON COMPOSITES FOR SODIUM-ION BATTERY ANODE APPLICATIONS

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Sodium-ion batteries and research about them have gained importance in the recent years due to supply chain and the cost problems of lithium-based batteries. The main drawback of sodium-based batteries is the fact that the theoretical capacity of sodium is lower than lithium due to its electrochemical performance [1]. In order to overcome that problem, many researchers have been looking into new anode materials that can work with sodium to increase the capacity of the whole battery.

One of the leading potential future anode materials for sodium-ion batteries is tin because of its high theoretical capacity [2]. Tin undergoes an alloying reaction with sodium instead of intercalation, that is one of the main reasons for its high theoretical capacity. But the main drawback is that when charged, tin containing electrode expands more than %400 volumetrically, which in turn damages the electrode. In order to overcome this problem, materials like carbon which have high structural durability have been used as composite additives with tin to work as a buffer and help with stability. Using sodium is more environmentally friendly than its alternative lithium for various reasons like mining. To make the cell more sustainable, anode side materials must be synthesized in a more environmentally friendly way as well. In this project, the anode material that is being used is tin oxide-carbon composite. Carbon in this material comes from the carbonization of plastic waste like polyethylene terephthalate (PET). Using recycled materials like PET helps to make the battery more sustainable.

The anode material is synthesized in a sealed pressurized reactor that operates at 700°C.

The final product is tin oxide particles covered with carbon that comes from carbonized PET. The main goal of this project is to upscale the direct pressurization reactor to produce this high-performance anode material in a mass scale. To achieve this, a sealed reactor with more than 400 ml of volume was designed with a construction material that could withstand 1000°C at 250 bars.

Key words: Reactor, Sodium-ion, Tin-Carbon Composites, Direct Pressurization, Sustainability

References

1. Biao Zhang, Gwenaëlle Rousse, Dominique Foix, Romain Dugas, Daniel Alves Dalla Corte, Jean-Marie Tarascon (2016). Microsized Sn as Advanced Anodes in Glyme-Based Electrolyte for Na-Ion Batteries. *Advanced Materials*, 9824-9830.
2. Zhi Li, Jia Ding, David Mitlin (2015). Tin and Tin Compounds for Sodium Ion Battery Anodes: Phase Transformations and Performance. *Accounts of Chemical Research*, 1657-1665.

HIGH CAPACITY, LONG LASTING, AND FAST CHARGING ORGANIC CATHODES FOR Li-ION BATTERIES

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Eliminating the use of critical transition metals in Li-ion battery cathodes is a key challenge for electrifying the transportation sector, especially in consumer vehicles. Vast resources are expended for replacing cobalt or minimizing the nickel content in commercial batteries, yet all rely on controlled doping of other elements (e.g. Mo, Mg, Ti, Mn, Nb) into ternary oxides to balance energy, power, safety, and cycling lives of such cathodes. An alternative strategy is to completely move away from inorganic oxides and use redox active organic materials, composed of just carbon, nitrogen, and oxygen, as cathodes. Despite the longstanding interest in developing organic cathodes, they generally perform poorly under practical conditions due to their relatively high solubility in battery electrolytes, which saps their cycle life, and low intrinsic electrical conductivity, which imposes needs for large amounts of additives and binders.

Here, we will describe the use of TAQ, a fused organic molecule with a layered structure that enables high electrical conductivity and complete insolubility in electrolytes, as a practically competitive cathode for Li-ion batteries. TAQ, made from just C, N, O, and H has higher energy density than incumbent commercial metal oxides at any charge-discharge rate, and maintains high capacity over thousands of cycles. It can deliver high charge capacity through reversible Li intercalation/de-intercalation between 2D molecular layers held together by a strong lattice of hydrogen bonds. Optimized electrodes made from TAQ outperform all commercial cathodes (including abundant lithium iron phosphate) at all charge-discharge rates, while retaining high capacity over thousands of cycles. Beyond the relevant battery metrics themselves, the structural and compositional principles underlining the electrochemical performance of TAQ provide a blueprint for the design and use of organic electrode materials in practical batteries.

Key words: organic batteries, sustainable cathodes, quinone

References

1. Chen, T.; Banda, H.; Wang, J.; Oppenheim, J. J.; Franceschi, A.; Dincă, M., A Layered Organic Cathode for High-Energy, Fast-Charging, and Long-Lasting Li-Ion Batteries, *ACS Central Science,* 2024, *10*, *569-578.*

MECHANISTIC INSIGHTS INTO ORGANIC ELECTRODE PERFORMANCE IN LITHIUM AND MAGNESIUM BATTERIES

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Redox-active organic electrodes, paired with high-energy metal anodes such as Li and Mg, represent a promising advancement toward sustainable energy solutions. However, the exact mechanisms at the particle level that control their operation are still largely unexplored. Furthermore, organic materials tend to exhibit a significant decline in electrochemical performance when transitioning to multivalent electrolytes, resulting in lower capacities, increased overpotentials, and worse rate performances [1].

In this study, a novel chemisorption mechanism is introduced to investigate the causes of these performance disparities using a model anthraquinone-based polymer in Li and Mg electrolytes. Through a combination of impedance spectroscopy and transmission line modeling based on the chemisorption model, we delineate the differences between the charge storage of Li and Mg ions and determine rate-limiting steps in both systems. The proposed model is validated by an array of techniques, including conductivity measurements, theoretical and experimental charge/discharge analyses, high-resolution EDX mapping, NMR studies, and DFT calculations.

Our comprehensive model accounts for processes across different time scales and provides a pathway for the systematic evaluation of organic electrode performance in different battery systems, with a particular focus on the challenges posed by multivalent chemistries.

Key words: redox-active organics, magnesium batteries, electrochemical impedance spectroscopy, electron microscopy.

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References

1. J. Bitenc, K. Pirnat, O. Luzanin, R. Dominko. Organic Cathodes, a Path toward Future Sustainable Batteries: Mirage or Realistic Future?, *Chem. Mater.*, 2024, vol. 36, pp. 1025-1040.

ELECTROACTIVE COORDINATION POLYMERS WITH PHOSPHONATE/ SULFONATE GROUPS FOR ENERGY STORAGE APPLICATIONS

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Sodium-ion batteries (SIBs) have emerged as promising alternative to lithium-ion batteries due to their low cost, environmental friendliness and resource availability [1] Coordination polymers (CPs) and metal-organic frameworks (MOFs), polymeric materials made up of metallic nodes and organic linkers, have gained interest as electrodes for energy storage applications due to their huge chemical and structural versatility. [2, 3] Redox-active anthraquinone (AQ) derivatives have been widely explored as building blocks for the synthesis of electroactive CPs and MOFs due to their high theoretical capacity and outstanding electrochemical reversibility. [1, 3, 4] Herein, we present the synthesis and characterization of two anthraquinone-based CPs explored as cathodes in SIBs. The aim was to study the electrochemical performance and cycling stability of the two redox-active CPs in SIBs to establish novel structure-performance relationships.

Key words: Redox-active CPs/MOFs; Na-ion Batteries, Anthraquinone.

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References

1. W. Tang, R. Liang, D. Li, Q. Yu, J. Hu, B. Cao, C. Fan. *ChemSushem* (2019), 12, 2181.
2. J. E. Halls, D. Jiang, A. D. Burrows, M. A. Kulandainathan, F. Marken. *SPR Electrochemistry* (2014), *12*, 187.
3. M. Souto, K. Strutyński, M. Melle-Franco, J. Rocha, *Chem. Eur. J.* (2020), *26*, 10912.
4. Z. Zhang, H. Yoshikawa, K. Awaga, *J. Am. Chem. Soc.* (2014), *136*, 16112.

REDOX POTENTIAL TUNING IN LITHIATED CARBOXYPHENOLATE-BASED ORGANIC ELECTRODE MATERIALS VIA CATION SUBSTITUTION

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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 materials. In fact, organic electrode compounds offer many interesting opportunities such as design flexibility and potentially lower cost and environmental burden [1]. 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., NMCs or $LiFePO_4$). For more than 15 years, our group has been working on both *n*- and *p-type* organic insertion materials with a special focus on the lithiated organic materials such as $Li_4C_6O_6$ [2] or Li_4-*p*-DHT [3]. Knowing the particularly good electrochemical performance of the latter compound upon cycling (a layered host structure), we have prepared a series of related materials based on the general formula $M^{n+}_{2/n}(Li_2)$-*p*-DHT ($M^{n+} = Mg^{2+}$, Ca^{2+}, Ba^{2+}, and Zn^{2+}) to probe the effect of the cation substitution commonly used with inorganic materials and pinpointed a quasilinear correlation between the average operating potential $<E>$ against the ionic potential (IP) of M^{n+}, the latter being formally a spectator cation [4,5]. A focus on the electrochemical performance of magnesium (2,5-dilithium-oxy)-terephthalate ($Mg(Li_2)$-*p*-DHT) and its electrochemical reaction mechanism will be done due to its pretty high operating potential (3.45 V vs. Li^+/Li).

Key words: organic battery, lithiated organic cathode, carboxyphenolate

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References

1. Poizot, P., Dolhem, F., *Energy Environ. Sci.*, 2011, 4, 2003–2019.

2. Chen, H., Armand, M. Courty, M., Jiang, M., Grey, C.P., Dolhem, F., Tarascon, J.-M., Poizot, P., *J. Am. Chem. Soc.*, 2009, 131, 8984–8988.
3. Renault, S., Gottis, S., Barrès, A.-L., Courty, M., Chauvet, O., Dolhem, F., Poizot, P., *Energy Environ. Sci*., 2013, 6, 2124–2133.
4. Jouhara, A., Dupré, N., Gaillot, A.-C., Guyomard, D., Dolhem, F., Poizot, P., *Nat. Commun*., 2018, 9, 4401.
5. Sajeevan, A. S., Bernard, L., Tran-Van, P., Brandell, D., Renault, S., Poizot, P., *ACS Appl. Polym. Mater.*, 2024, 6, 10102–10112.

AMELIORATING THE NICKEL-RICH CATHODE/SULFIDE SOLID-STATE ELECTROLYTE INTERFACE STABILITY BY THE ORGANIC/INORGANIC DUAL COATING

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LPSC-type sulfide solid-state electrolytes ($Li_{6-x}PS_{5-x}Cl_{1+x}$) with high ionic conductivity are regarded as crucial materials for the next generation of high-energy-density, high-safety batteries. However, the layered cathode materials selected to achieve high energy density present numerous interfacial challenges, including electrochemical and mechanical stability issues. In this study, we have employed a dual-coating approach utilizing ionically conductive and electrochemically stable inorganic/organic materials to mitigate interfacial space charge layer effects and enhance cycling stability.

Organic polymers typically exhibit excellent interfacial stability but are often limited in their applicability to liquid/polymer solid-state batteries due to their solubility in polar solvents and relatively low electrical conductivity. The novel and effective strategy of combining stable and conductive poly (vinylene carbonate) with highly conductive LPSC addresses these limitations. Uncoated samples in sulfide solid-state batteries paired with stable lithium-indium anodes demonstrate a discharge capacity of only approximately 120 mAh/g at 1 C. By coating the sulfide solid-state electrolyte (LVC3) with the polymer solid electrolyte poly (vinylene carbonate), charge transfer between the electrode and electrolyte is significantly optimized, resulting in an increased discharge capacity of about 150 mAh/g at 1 C. Furthermore, most oxygen-containing organic compounds tend to over-associate with lithium in sulfide solid-state electrolytes, impeding ion conduction. To address this issue, ionically conductive lithium borate is employed on the cathode surface to alleviate the space charge layer effect. Simultaneously, polyvinylpyrrolidone is uniformly dispersed and anchored to the transition metal oxide surface, ensuring mechanical and chemical stability during cathode cycling. Upon completion of this dual-coating process, the battery's rate performance is further enhanced, achieving a discharge capacity of approximately 170 mAh/g at 1C. Moreover, in full cells paired with micrometer-sized silicon, a capacity of 4 mAh/cm^2 is maintained with remarkable stability after 80 cycles at a current density of 1 mA/cm^2.

This comprehensive approach for interface engineering demonstrates significant improvements in the performance and stability of solid-state batteries, paving the way for the development of high-energy-density energy storage systems with enhanced safety and longevity.

Key words: Organic/inorganic dual coating; Nickel-rich cathode; Sulfide solid-state electrolyte; Space charge layer; Mechanical stability.

References

1. Chen, H. et al., *Phys. Chem. Chem. Phys.,* 2015, 17, 16494.
2. Shi, B. et al. *Adv. Energy Mater.,* 2023, *13*, 2300310.
3. Wang, S. et al. *ACS Nano,* 2022, 16, 16158.
4. Yang, X. et al., *Angew. Chem.,* 2023, 135, e202215680.
5. Yuan, H. et al., *Nano Energy,* 2024, 128, 109835.

DEVELOPMENT OF MULTIVALENT ELECTROLYTES BASED ON FLUORINATED ALKOXYBORATE AND ALKOXYALUMINATE SALTS

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Multivalent Mg and Ca batteries offer a promising avenue to the development of next-generation batteries based on abundant materials. The high gravimetric and volumetric capacities of Mg (2206 mAh/g, 3834 mAh/cm^3) and Ca (1337 mAh/g, 2073 mAh/cm^3) metal anodes enable development of high-energy density battery cells that could either replace or complement current Li-ion battery technology. Mg and Ca battery research currently faces two challenges: There is lack of suitable electrolytes and cathode materials.

The problems with electrolytes are mainly related to the difficult dissociation of multivalent salts as well as insufficient reductive and oxidative stability and limited metal plating/stripping efficiency. While the development of Mg electrolytes has started in 1990s, significant progress has been made in the recent years with the introduction of new salts based on weakly coordinating anions which are characterized by good compatibility with a variety of cathode materials. In our work, we investigated the influence of fluorinated alkoxy ligands on the properties of Mg electrolytes as well as the influence of Mg salt concentration. We have shown that the salt synthesis process has a key influence on both the purity and the electrochemical performance of the salts. Additionally, we have investigated the effect of different additives on Mg metal/plating process. [1,2] Furthermore, the improved electrochemical performance of aluminate-based salts has also been showcased also on the case of Ca electrolytes. [3] At the same time, we also take a look at the performance of different cathode materials in new multivalent electrolytes.

Key words: Multivalent batteries, electrolytes, weakly coordinating anions, metal plating/stripping

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References

1. Pavčnik, T. *et al.* On the Practical Applications of the Magnesium Fluorinated Alkoxyaluminate Electrolyte in Mg Battery Cells. *ACS Appl. Mater. Interfaces,* 14, 26766-26774 (2022).
2. Pavčnik, T., Imperl, J., Kolar, M., Dominko, R. & Bitenc, J. Evaluating the synthesis of Mg[Al(hfip) 4] 2 electrolyte for Mg rechargeable batteries: purity, electrochemical performance and costs. *J. Mater. Chem. A,* 12, 3386-3397 (2024).
3. Pavčnik, T. *et al.* A novel calcium fluorinated alkoxyaluminate salt as a next step towards Ca metal anode rechargeable batteries. *J. Mater. Chem. A,* 11, 14738–14747 (2023).

ELECTRODES BASED ON METAL-ORGANIC FRAMEWORKS FOR ANODE-LESS Na-ION RECHARGEABLE BATTERIES

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Nowadays, sodium-ion batteries (NIBs) are gaining attention as a potential alternative to lithium-ion batteries (LIBs). The finite availability of lithium, mainly concentrated in limited geographical regions, has raised economic and social concerns regarding its extraction, instead, sodium is the most abundant alkali metal in the Earth's crust, offering a promising and cheaper alternative. [1] However, the larger atomic radius of sodium compared to lithium requires the exploration of novel electrode materials capable of significant structural variation to accommodate sodium ions, and thus posing challenges in achieving comparable energy density. [2]

Anode-less batteries are a promising technology that could help to achieve high energy densities and reduce total cell weight.

This study investigates the feasibility of addressing the energy density challenge in sodium chemistry through an anode-less architecture, enabled using a zinc-based metal-organic framework (MOF) to realize sodiophilic current collectors (SCC).

Zinc 4^{l},4 bipyrazole was synthesized as previously reported in literature [3], mixed with conductive carbon and casted onto aluminium foil to obtain a conductive thin film. Different concentration of MOF and the use of additive were evaluated.

The electrochemical performances of the so obtained sodiophilic electrodes were first evaluated in half cell configuration (SCC/electrolyte/Na), in particular, the nucleation energy and the stability of the system were studied through stripping and plating deposition tests. Remarkably, an efficiency of almost 100% is still maintained for at least 700 cycles, making the SCC a promising candidate for further practical applications.

A Prussian Blue (PB) was synthesized, fully characterized and employed as cathodic material for the full cell configuration (SCC/electrolyte/PB) which was successfully assembled, moreover, the cycling performance as well as the rate capability of the full cell were investigated using GCPL technique.

In conclusion, the results suggest favourable compatibility between the PB cathode and the sodiophilic current collector, enabling a notably high specific capacity, minimal capacity fade, remarkable energy densities, and robust stability even under increasing current densities.

Key words: Na-ion batteries, anode-less battery, metal-organic frameworks, Prussian Blue analogues.

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References

1. Li, H. et al. (2022). Sodiophilic Current Collectors Based on MOF-Derived Nanocomposites for Anode-Less Na-Metal Batteries. *Advanced Energy Materials*, DOI: 10.1002/aenm.202202293.
2. Cohn, A.P. et al. (2017). Anode-Free Sodium Battery through in Situ Plating of Sodium Metal. *Nano Letters*, DOI: 10.1021/acs.nanolett.6b05174.
3. Pettinari, C. et al. (2012). Novel coordination frameworks incorporating the 4,4′-bipyrazolyl ditopic ligand. *Inorganic Chemistry*, DOI: 10.1021/ic3001416.

THE CHEMISTRY EUROPE JOURNALS AND PUBLISHING OPEN ACCESS

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Chemistry Europe is an association of 16 European chemical societies from 15 European countries. It publishes a family of high-quality scholarly chemistry journals, covering a very broad range of disciplines. In this talk, we will give a short overview of Chemistry Europe, their mission, their journals, and how the editorial office operates. After this, we will provide a brief introduction to publishing open access, including a comparison of the different types of open access, the advantages of publishing open access as well as Wiley's approach and our transformational agreements.

BATTERY MANUFACTURING: FROM DIGITAL MODELS TO DIGITAL TWINS

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In this lecture I first discuss the concepts of digital model, digital shadow and digital twin and how they can be used to optimize battery electrodes and cell design and their manufacturing process. Different types of pioneering digital models developed in my research group, coupling numerical simulations with AI, are presented, with illustrative application examples arising from my past and ongoing research projects, such as the ERC-funded ARTISTIC (https://www.erc-artistic.eu/). Illustrations disclosed are about lithium ion, sodium ion and solid-state battery electrodes, prepared with wet and dry processing. Methodologies to ensure the proper experimental calibration and validation of these digital models are also discussed. I also present our Virtual and Mixed Reality tools designed to support the training of students, researchers and operators in the battery manufacturing field. Finally, I briefly introduce a startup, originating from my 10 years work in the field of digitalization of battery manufacturing processes, that gives the promise to be a game changer.

Key words: battery manufacturing, materials processing, computational modeling, artificial intelligence, optimization, digital twins

EVOLUTION OF Li-METAL ELECTRODES ANALYZED VIA CLUSTERING DATA–MINING METHODS

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Symmetric Li||Li cells are commonly used to investigate the behavior of Li-metal anodes in Li-metal batteries (LMBs) and the compatibility of a given electrolyte in contact with Li metal. The voltage trace during such stripping/plating experiments is a very sensitive indicator of the electrochemical processes and morphological changes occurring in the cell. However, the eventual changes during each single cycle are often subtle, making it challenging to track long-term alterations. Additionally, the vast amount of data complicates a comprehensive understanding of the evolution over the entire cycle life via a manual comparison.

To address this issue, we developed a data-mining clustering method to identify cycle patterns and extract hidden information from the extensive datasets. This unsupervised machine learning method enables the objective separation of the evolution process based on the similarity between voltage traces of individual stripping/plating cycles. Based on the analysis of a large quantity of experimental data, we propose a four-cluster stage model for Li-metal anodes, correlating with the formation of dead Li and pits in the early stages and the accumulation of the Li deposition layer during subsequent cycle stages.

We further validated the similarity of cluster stages under different conditions using in situ optical microscopy and SEM, confirming the rationale of the four-cluster stage model and our data-mining approach. This data-mining method has the potential to provide new insights by evaluating extensive cycling datasets and to enhance our understanding of the relevant impact factors for achieving long-term stable Li-metal anodes and electrolytes.

Key words: Li metal batteries (LMB), Li-metal anodes, Data-mining clustering, Machine learning method, Electrochemical process.

TAILORING CATHODE MATERIALS: INNOVATIVE HYBRID HIGH VOLTAGE ELECTRODES BASED ON *LMNO/LFP* FOR NEXT-GENERATION LiBs

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Electrochemical energy-storage systems, such as lithium-ion batteries (LiBs), have turned out to be the most prevalent technology for a wide range of devices, from small electronics to stationary energy storage applications, and electric mobility. However, to meet the ever-increasing market demand, significant effort is still needed in order to develop batteries with better performance in terms of power and energy density.

In this frame, cathode materials completely cobalt-free and operating at high voltage, such as LNMO ($LiNi_{0.5}Mn_{1.5}O_4$) are particularly interesting and potentially able to increase the electrochemical performance of next-generation high-energy-density LiBs.

Unfortunately, LNMO still suffers of some drawbacks such as easy cation leaching during cycling and electrolyte decomposition at high voltage. Therefore, one possible approach to mitigate these issues, increasing the safety of the system, the lifetime, and limiting the cost, is using blended electrodes, containing multiple types of active materials.

In the present work, within HYDRA H2020 project, the influence of LFP ($LiFePO_4$) physically mixed with LMNO was studied both from morphological and electrochemical point of view. LFP was chosen because of its outstanding thermal and electrochemical stability, and its cycling performances, lifetime and safety. The role of LFP was studied changing its amount inside the cathode formulation and the electrochemical properties were evaluated both in half-cell and full-cell configuration.

In particular, the simple and up-scalable physical blending, by resonant acoustic mixing (RAM) technique, provided a good distribution of LFP and LNMO particles, resulting in increased electrochemical performances. The blended LNMO/LFP cathode delivered a specific capacity > 125 mAh g^{-1} at C/10 and a capacity retention > 80% after 1000 cycles at 1C. Analogously, the blended electrode showed a capacity retention of 74% after 100 cycles in full-cell configuration, almost 30% higher than the pure LNMO cathode [1].

Key words: LIBs, Cathode, LNMO/LFP blended, Energy density, Cycling stability

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References

1. Versaci, D., et al., Journal of Power Sources, 613, 234955, 2024

APPLICATION OF SMART FUNCTIONALITIES IN BATTERIES

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The increasing reliance on batteries requires closer monitoring of battery health and safety to increase their reliability and lifespan. Li-ion cells are susceptible to various degradation mechanisms. Among them, the inventory loss of lithium through irreversible reactions and the dissolution of transition metals appears to be one of the main causes of capacity and performance degradation. The initial loss of lithium in the formation cycle can be replaced by the pre-lithiation step, while the later degradation processes lead to a continuous loss of lithium. This is partly caused by the dissolution of transition metals from the cathode material and leads to an additional capacity drop, mainly caused by the need for additional passivation when the transition metals on the negative electrode are reduced.

The dissolution of transition metals can be partially monitored by external parameters as the dissolved cations are deposited on the negative electrode where they are reduced, requiring the growth of a passive film which is reflected in the increase in polarization.

A step forward in the control and understanding of cell degradation would be possible through in- built sensor systems that allow the collection of various information during battery operation. The sensor technologies should be designed to monitor the most damaging process for the battery cell.

In this paper, we show how the advances that have been made in the field of printed electronics can be applied to Li-ion batteries. To do this, we use an electrochemical sensor that reliably detects manganese ions in the early stages of manganese dissolution. We also show a possible strategy for the regeneration of Li-ion batteries.

Two intelligent functions integrated into the battery cells can improve the quality, reliability, service life and safety of future Li-ion batteries.

Key words: printed sensor, transition metal dissolution, loss of lithium, passivation, batteries

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References

1. PALJK, Tina, BRACAMONTE, Victoria, SYROVY, Tomas, DRVARIČ TALIAN, Sara, HOČEVAR, Samo B., DOMINKO, Robert. Integrated sensor printed on the separator enabling the detection of dissolved manganese ions in the battery cell. Energy storage materials. Jan. 2023, vol. 55, str. 55-63.
2. DOMINKO, Robert, PALJK, Tina, BRACAMONTE, Victoria, SYROVY, Tomas, Electrochemical sensor based on printed circuits enabling detection of soluble cations in the battery cell, Patent Application PCT/EP2022/052352

MOLECULAR-BASED CONDUCTIVE ACTIVE MATERIAL FOR METAL-ION BATTERIES

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Utilizing organic materials in battery technologies provides numerous advantages, including enhanced durability and cost-effectiveness related to the abundance of their constituents. They also offer a remarkable degree of versatility in shaping their structural design. Nevertheless, in the current development of batteries, these electro-active materials encounter a major challenge: their electronic conductivity. The deficiency in conductivity leads to low electrochemical performances and requires a high amount of conductive carbon (20-60 wt%). This high amount of additive lowers the quantity of active material in the electrode and diminishes drastically the energy density.

Over the past decades, various strategies have been explored in order to face this challenge, such as organized molecular systems [1, 2] or metal-organic active materials [3]. Very recently, charge transfer complexes based on TTF-TCNQ [4] has also been investigated as electroactive material and has gained attention for their high electronic conductivity up to 300 S/cm.

In this context, our work focuses on the development of new molecular redox active materials for ion batteries with high electronic conductivity to lower the amount of carbon additive and maximize storage performances. In such approach, we had a look at radical salt generated by electro-crystallization and presenting an electronic conductivity reaching 0.05 S/cm at 300 K. Galvanostatic cycling and full material characterization are in the center of the study. A specific attention has been paid to advanced characterization of the material at different state of oxidation/reduction such as X-ray operando and Electrochemical Impedance Spectroscopy to investigate the behavior of this new active material in batteries.

Key words: Organic active material, high electronic conductivity, positive electrode, sodium-ion.

References

1. V. Pignier, S. Toumieux, C. Davoisne, M. Caroff, A. Jamali, S. Pilard, D. Mathiron, D. Cailleu, F. Delattre, D.P. Singh, R. Douali, M. Becuwe, *Small,* (2023), 2305701.
2. É. Deunf, P. Moreau, É. Quarez, D. Guyomard, F. Dolhem, P. Poizot, *J. Mater. Chem. A*, 4 (2016), p. 6131-6139.
3. C. Fang, Y. Huang, L. Yuan, Y. Liu, W. Chen, Y. Huang, K. Chen, J. Han, Q. Liu, Y. Huang, *Angew Chem Int Ed*, 56 (2017), p. 6793-6797.
4. Y. Fujihara, H. Kobayashi, S. Takaishi, T. Tomai, M. Yamashita, I. Honma, *ACS Appl. Mater. Interfaces*, 12 (2020), p. 25748-25755

FUNCTIONAL BINDERS TO ADDRESS TRANSITION METAL DISSOLUTION IN *LNMO* CATHODE MATERIAL

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$LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) is a high-voltage spinel oxide that stands out as a highly promising cathode material for next-generation lithium-ion batteries, particularly in electric vehicles. With an operating voltage around 4.7 V (vs. Li/Li^+), LNMO provides a significant energy density of approximately 650 Wh/kg, combined with exceptional high-rate performance, making it an ideal candidate for applications requiring rapid charging and discharging. The use of nickel and manganese, which are both abundant and cost-effective, further enhances the material's appeal from an economic and sustainability perspective [1].

Despite these advantages, the practical implementation of LNMO in commercial batteries faces several challenges. One of the primary issues is the material's interaction with the electrolyte at high voltages. When exposed to these conditions, the electrolyte can oxidize, particularly in the presence of moisture, leading to the formation of hydrofluoric acid (HF). HF is highly corrosive and can cause the dissolution of Mn^{2+} ions from the LNMO cathode. Once dissolved, these Mn^{2+} ions can migrate through the electrolyte to the Solid Electrolyte Interphase (SEI), where they are reduced to metallic state. This deposition not only increases the internal resistance of the battery but also contributes to the gradual degradation of capacity, significantly impacting the long-term performance and cycle life of the battery. Furthermore, the presence of metallic Mn on the anode can catalyze further decomposition of the electrolyte, posing a substantial barrier to the adoption of LNMO-based batteries [2].

This study is part of the ongoing European project IntelLiGent, which aims to develop non-fluorinated binders for LNMO that incorporate metal-ion scavengers to address these challenges. The goal is to capture dissolved transition metal ions before they reach the anode interface, thus preventing potential damage. Another key objective is to enhance the aqueous processability of LNMO. To achieve these goals, various binders, including lithiated biopolymers with different molecular weights, and lithiated technical polymers at varying pH values were examined. The results of electrochemical cycling reveal a strong dependence on the functionality of the binders, influenced by both molecular weight (Mw) and pH levels.

Key words: High-voltage cathode material, LNMO, Cycling stability.

Acknowledgments *(if applicable)*
IntelLigent has received funding from the European Union's Horizon Europe research and innovation program, under grant agreement No 101069765. Marit Sandrød (SINTEF), is acknowledged for obtaining ICP-MS data.

References

1. Kim, J et al. C*hemPhysChem*, 15: 1940-1954 (2014).
2. Zhan, C et al. *Nat Commun* 4, 2437 (2013).

INTERFACE AND INTERPHASE IN CALCIUM AND MAGNESIUM METAL ANODE BATTERIES

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Various metals have been used as battery anodes in electrochemical cells ever since the birth of the batteries with Volta's pile and in the first commercialized primary (Zn/MnO_2, Leclanché 1866) and secondary (Pb/acid, Planté 1859) batteries. Li-MoS_2 cells, employing Li metal anodes, with specific energies two to three times higher than both Ni/Cd and Pb/acid cells, were withdrawn from the market due to safety issues related to dendrites growth. Instead, electrodeposition of Mg and Ca appears to be less prone to dendrite formation. [1, 2] Pioneering work by Aurbach et al. in the early 1990's showed a surface-film controlled electrochemical behavior of Ca and Mg metal anodes in electrolytes with conventional organic solvents. [3, 4] The lack of metal plating was attributed to the poor divalent cation migration through the passivation layer.

Nevertheless, recent demonstration of Ca and Mg plating and stripping in the presence of a passivation layer or an artificial interphase [2, 5, 6] has paved the way for assessment of new electrolyte formulations with high resilience towards oxidation. However, several challenges remain to be tackled for the development of Ca and Mg based batteries. [7, 8] Among these, the need for reliable electrochemical test protocols, mass transport limitations and high desolvation energies (due to strong cation-solvent and cation–anion interactions) are implied. [9, 10] Here, the reliability of electrochemical set-ups involving multivalent chemistries is discussed, and a systematic investigation on the impact of the electrolyte formulation on the cation solvation structure and transport is presented. A systematic characterization of the SEI formed on the Ca metal anode in various electrolyte formulations using complementary techniques allowed for the identification of the most suitable SEI compounds in terms of divalent cation mobility. [11] Finally, recent development on cathode materials will be discussed including promising organic cathode materials. [12]

Key words: Post-Li, electrolyte, solid electrolyte interphase, interface, metal anode

References

1. M. Matsui, *J. Power Sources*, 196 (2011) 7048
2. A. Ponrouch, C. Frontera, F. Bardé, M.R. Palacín, *Nat. Mater.*, 15 (2016) 169
3. D. Aurbach, R. Skaletsky, Y. Gofer, *J. Electrochem. Soc.*138 (1991) 3536
4. Z. Lu, A. Schechter, M. Moshkovich, D. Aurbach, *J. Electroanal. Chem.* 466 (1999) 203
5. D. Wang, X. Gao, Y. Chen, L. Jin, C. Kuss, P. G. Bruce, *Nat. Mater.* 17 (2018) 16
6. S.-B. Son, T. Gao, S. P. Harvey, K. X. Steirer, A. Stokes, A. Norman, C. Wang, A. Cresce, K. Xu, C. Ban, *Nat. Chem.* 10 (2018) 532

7. J. D. Forero-Saboya, D. Tchitchekova, P. Johansson, M.R. Palacín, A. Ponrouch*, Adv. Mater. Interfaces*, 9 (2022) 2101578
8. A. Ponrouch, J. Bitenc, R. Dominko, N. Lindahl, P. Johansson, M.R. Palacín, *Energy Stor. Mater.* 20 (2019) 253
9. D. S. Tchitchekova, D. Monti, P. Johansson, F. Bardé, A. Randon-Vitanova, M. R. Palacín, A. Ponrouch, *J. Electrochem. Soc*., 164 (2017) A1384
10. R. Dugas, J. D. Forero Saboya, A. Ponrouch, *Chem. Mater*., 31 (2019) 8613
11. J. D. Forero-Saboya, C. Davoisne, R. Dedryvère, I. Yousef, P. Canepa, A. Ponrouch, *Energy Environm. Sci.* 13 (2020) 3423
12. D. Monti, N. Patil, A. P. Black, D. Raptis, A. Mavrandonakis, G. E. Froudakis, I. Yousef, N. Goujon, D. Mecerreyes, R. Marcilla, A. Ponrouch, *ACS Appl. Energy Mater*. 6 (2023) 7250

SOLVENT-FREE EXTRUSION OF POLYMER ELECTOLYTES FOR ALL-SOLID-STATE BATTERIES

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Solid-State Batteries (SSB) are intensely investigated in the research of high energy densities and safety. Among them, polymer-based materials are attractive regarding their cost and high potential for upscale. As electrolytes, polymers manage to create good interfaces with the electrodes, a common difficulty in the SSB field. The main drawback of Solid Polymer Electrolytes (SPE) is generally their limited ionic conductivities. In this study, we aimed at producing a high voltage operating SPE, based on conductive polymers and polymeric salts. An emphasis was given to the production method and shaping of the electrolyte, involving processes with a good upscale potential.

Different electrolytes were formulated varying the nature and relative proportions of conductive polymers, lithium salts and additives, without use of any solvent. A Single-Ion Conducting Polymer (SICP) was used to obtain high values of transference number. Electrolyte films were produced with an extrusion process, fine-tuned for each formulation to create soft conditions and avoid degradation. The SPEs were studied through thermal analyses (TGA, DSC), and their ionic conductivities measured with EIS. This work highlights the performance of fully extrudable SPEs and the use of SICP in SPEs formulations, with an insight on the limitations of such systems.

Key words: solid-state-batteries, polymer electrolyte, solvent-free extrusion, single-ion conducting polymer.

NOVEL SINGLE-ION CONDUCTING POLYMER ELECTROLYTE FOR LITHIUM-METAL BATTERIES

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In recent years, solid-state lithium-metal batteries (SSLMBs) have attracted a continuously increasing attention owing to the promise of higher energy density than state-of-the-art lithium-ion batteries comprising a liquid electrolyte [1]. Specifically, single-ion conducting polymer electrolytes (SIPEs), in which the ionic function is covalently tethered to the polymer backbone, have recently been studied intensively [2, 3]. In this work, a polyamide-based single-ion conducting polymer electrolyte was developed via a simple radical chain polymerization using an allyl-based cross-linking agent, and a (trifluoromethanesulfonyl)imide-type ionic function. The design of the polymer skeleton is enriched with abundant polar groups, which provides a high number of potential coordination sites for the Li+ cations, thus, supporting a rapid and uniform charge transport. When blended with a polymer that provides suitable mechanical properties and small molecules with a high dielectric constant, self-standing and flexible polymer electrolyte membranes are obtained, with a high ionic conductivity of 1.1×10^{-4} S cm^{-1} at room temperature and a high electrochemical stability towards oxidation of up to about 4.8 V. As a result, symmetric Li││Li cells containing this novel electrolyte show a very stable stripping/plating for more than 1,800 h and Li||$LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$ as well as Li||$LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ cells provide very good cycling stability and rate capability, rendering this single-ion conductor very promising for next-generation SSLMBs.

References

1. Toon, K. et al. Challenges and Strategies towards Practically Feasible Solid-State Lithium Metal Batteries. *Adv. Mater*. 34, 2104666 (2022).
2. Lopez, J. et al. Designing polymers for advanced battery chemistries. *Nat. Rev. Mater.* 4, 312–330 (2019).
3. Zhu, J. et al. Single-Ion Conducting Polymer Electrolytes for Solid-State Lithium–Metal Batteries: Design, Performance, and Challenges. *Adv. Energy Mater.* 11, 2003836 (2021).

INVESTIGATION OF VOLATILE ELECTROLYTE DECOMPOSITION PRODUCTS WITH OPERANDO *GCMS* FOR LITHIUM-ION BATTERIES

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For decades, great efforts have been devoted to Lithium-Ion Batteries (LIBs) with the goal to improve performance and further strengthen their market position in mobile and grid energy storage applications. The liquid electrolyte, which is a key component of the battery, undergoes decomposition during cell operation to form a protective layer mainly on the anode. This solid electrolyte interphase (SEI) layer prevents further electrolyte reduction and is crucial for enhancing cell lifetime and safety. The most common strategy to form a stable passivation layer is to use SEI forming additives which are prone to polymerize in a rapid and controlled manner. [1]

Commonly used electrolytes consist of organic carbonate-based solvents and an inorganic salt, which decompose during cycling to form the SEI. Some side products are volatile and result in a complex mixture of gases. Understanding the decomposition processes leading to gas species evolution and the formation of a stable SEI is a topic which has attracted increased interest in the research community. While volatile components can be identified by means of gas analysis, non-soluble compounds precipitate on the electrode surface and are commonly analysed with surface sensitive techniques, such as X-ray photoelectron spectroscopy (XPS). Combining gas analysis with XPS gives a more comprehensive insight in electrolyte decomposition and the formation of passivation layers.

In this work, we present the evolution of volatile components during the first formation cycle in a LIB. Standard carbonate-based electrolytes containing the SEI-forming additives fluoroethylene carbonate (FEC) and vinylene carbonate (VC) were investigated. Pouch cells and laboratory-scale coin cells were subjected to operando GC/MS experiments and evolved gas species measured in conjunction with the cell potential.

The study revealed that, in addition to major gaseous components such as CO, CO_2, methane, ethane, and ethene, a variety of C_3 to C_6 hydrocarbons, ethers, and carbonyls were observed. Particular attention was given to decomposition products related to the degradation of $LiPF_6$. The analysis showed that the complex gas mixture consists of carbonate components originating from transesterification reactions and evaporation of the volatile electrolyte. Inorganic components such as carbon monoxide and carbon dioxide were found to mainly stem from the degradation of cyclic carbonates, while saturated and unsaturated hydrocarbons were attributed to the linear carbonate components, as well as ether and carbonyl compounds. Results from gas analysis were compared with XPS data of extracted electrodes and correlated with decomposition pathways of the electrolyte.

Key words: Lithium-ion batteries, electrolyte decomposition, additives, SEI, CEI, operando GCMS.

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References

1. Qian, Y. et al. Investigations on the electrochemical decomposition of the electrolyte additive vinylene carbonate in Li metal half cells and lithium-ion full cells. J. Power Sources 332, 60–71 (2016).

INVESTIGATION OF REACTIVITY AND DEGRADATION MECHANISMS OF Na_2NDC NEGATIVE ORGANIC ELECTRODE MATERIAL BY *TEM* AND *OPERANDO XRD*

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The growing demand for electric batteries poses the challenges of resource scarcity. The use of organic electrode materials could release the strain on metal extraction in addition to being easily recyclable and having low-cost chemically adaptable structures [3].

The sodium salt of 2,6-naphthalene dicarboxylic acid (Na_2NDC) is a promising material as negative electrode for sodium-ion battery owing to its low potential of 0.4V *vs* Na and high-rate capability [1]. Recently, Na_2-NDC was integrated in a sodium-ion hybrid full cell (associated with NVPF) displaying 155Wh/kg after 400 cycles. However, it was shown that both electrolyte and electrode material were degrading during cycling which led to long term capacity fading due to unclear phenomenon [4]. Hence, in-depth investigation of Na_2NDC degradation and electrochemical reactivity during cycling is necessary to improve the cell performance.

Cryogenic Transmission Electron Microscopy (Cryo-TEM) and its associated techniques (electron diffraction, electron energy loss spectroscopy) are powerful tools to provide structural, microstructural and chemical data that can be used to elucidate reactivity mechanisms and identify material and interface degradation [2]. Coupled with *operando* X-Ray Diffraction, investigation on electrode material at different state of charge during the first cycles were carried out. Thanks to this approach, structural, microstructural and morphological changes during cycling were observed, opening the way toward the full understanding of the degradation mechanisms involved.

To understand the impact of the structure on Na2NDC electrochemistry, the synthesis procedure was adapted to obtain amorphous particles. Their electrochemical behaviour was then investigated and suggest that electrochemical performance can be modulated and improved as a function of textural properties.

Key words: Organic electrode, electron microscopy, *operando* X-Ray Diffraction

References

1. J.M. Cabañero & Al, ChemSusChem, 12, p. 4522–4528, (2019)
2. C. Davoisne & Al, Journal of The Electrochemical Society, 164 (7) A1520-A1525 (2017)
3. P. Poizot, Chemical Reviews, 120 (14), p. 6490-6557, (2020)
4. R. Russo, Sustainable Materials and Technologies, (2023), Volume 36, 2214-9937

THE DIGITAL EDGE: HOW DATA DRIVES BATTERY BREAKTHROUGHS

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Battery research and innovation creates vast amounts of data. This data comes from many different sources including testing, simulation, and management systems. Although it has enormous potential, battery data is often under-utilized because of inconsistent structuring and a lack of descriptive metadata. This talk explores how the structuring, annotating, and linking of battery data can significantly accelerate battery research and innovation activities and lead to new knowledge.

The recent development of standardized data models with semantic annotations has made battery data machine-readable and interoperable. This facilitates improved traceability and integration across different platforms and frameworks. Linked data techniques enable the creation of knowledge graphs, which support automated workflows and uncover new relationships between data points, materials, and components [1]. This structured approach can reduce manual intervention and improve data-driven insights, leading to more efficient operations and decision-making processes.

In parallel, linked data provides a critical foundation for advancing battery modeling. Modern battery models have seen dramatic improvements in both speed and accuracy, but they still face challenges in data integration. Linked data pipelines can be used to efficiently feed modelling frameworks with data for both parameterization and validation workflows. This can help to automate some aspects of battery simulations and accelerate the overall design process.

This presentation highlights how the combination of structured battery data and advanced models can push the boundaries of battery research. By bridging the gap between data and modeling, we unlock the potential for faster and more reliable insights, ultimately driving innovation and breakthroughs in battery technology. Real world use-cases demonstrating the practical implementation of these techniques will be discussed, along with the challenges and future directions for research in this field.

Key words: battery, digitalization, linked-data, analytics, simulation

Acknowledgments

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References

1. S. Clark *et al.*, Toward a Unified Description of Battery Data, *Adv Energy Mater*, vol. 2102702, 2021, doi: 10.1002/aenm.202102702.

TOWARDS GREENER ENERGY STORAGE SOLUTIONS: BIORENEWABLE ORGANOGELS FOR Li-O_2 BATTERIES

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The growing need for clean energy production, due to global warming, has addressed the research towards the study of cleaner and more performing energy storage solutions and electric vehicles technologies. One of the most promising technologies currently being studied is the lithium – oxygen (Li-O_2) battery, thanks to its high theoretical energy density of the order of 11000 Wh kg^{-1}. This extraordinary value is explained by the use of a metallic lithium anode but, above all, by the use of porous carbon cathodes (GDL) where the active material, oxygen, flows from the outside. The use of metallic lithium anodes, however, results in many drawbacks that limit the stability and cycling of these batteries. For this reason, in this work, biorenewable organogel membranes have been studied to enhance this system performances using green solutions.

The two main building blocks employed in the reported studies are gelatin, extracted from cold water fish skin, and chitosan which is derived from the deacetylation of chitin, the second most abundant polymer in nature after cellulose. Both gelatin and chitin (from shrimp and crab shells) can be obtained from the fish industry waste, as such they are cheap, abundant, as well as green, biorenewable and biocompatible polymers. Another common point between these two molecules is that they can easily be methacrylated using a single step reaction in water, allowing their successive cross-linking through UV-initiated free radical polymerization, thus obtaining organogels with interesting mechanical properties. For example, these organogels can be activated with common liquid electrolytes to obtain green gel polymer electrolytes (GPEs). Moreover, the mechanical properties can be further enhanced using yet another element obtained from industry waste, a wood flour which is as well methacrylated and act as reinforcing filler within the gelatin based GPE.

These different GPEs formulations were tested in Li-O_2 cells and the obtained performance were compared to the ones of cells assembled with commercial separators and liquid electrolytes. Interestingly, it was observed that the increase in cycle life could be explained in the three studies by a modification of the reaction mechanism between lithium and oxygen resulting in more amorphous lithium peroxide deposition and therefore an increased system reversibility.

Key words: lithium-oxygen battery; gel polymer electrolyte; photopolymerization; bio-renewable resources; chitosan; gelatin; wood flour.

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RECYCLE PLASTIC WASTE FOR THE APPLICATION ENERGY STORAGE

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Recently, many kinds of plastics are widely used in all of the world, which are mainly composed of carbon and hydrogen element. However, “white pollution” is becoming more and more serious due to the accumulation of waste plastics on land and in ocean. It is a great challenge to recycle these plastic wastes due to the chemical stability of plastic in nature. Because the traditional way does not fully take use of the polymer and induces environmental concerns, it is highly urgent to develop an environmental friendly way to recycle plastics waste to high-value-added products. Carbonization plastic waste is one choice due to the wide applications of carbon materials. With this method, we have developed a series of ways to produce carbon materials from plastic wastes. More importantly, the obtained carbon nanomaterials were used in lithium-ion batteries and supercapacitors. In another way, converting plastic waste into MOFs and using the resulting MOFs as OER catalyst is also presented. The results prove it is a cost effective way for the recycling of plastic waste into high value-added products. These results pave a potential way to upcycle plastic wastes into valuable products.

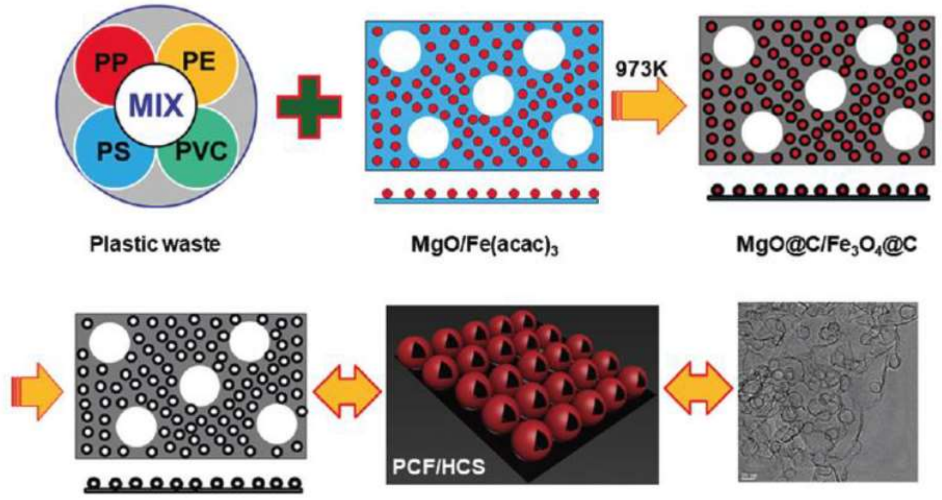

Fig. 1: *Recycle plastic waste into carbon nanomaterials and application in lithium ion battery*

Key words: Plastic waste, supercapacitor, lithium ion battery, carbon nanomaterials

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HIGH VOLTAGE SPINEL OXIDE AS CATHODE MATERIAL FOR Li-ION BATTERIES

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This study explores the synthesis and electrochemical characterization of Lithium Copper Manganese Oxide (LCMO) as a high-voltage cathode material for lithium-ion batteries. Conducted in collaboration with the Commissariat à l'énergie atomique (CEA)-LITEN in Grenoble, the research aims to elucidate the lithiation mechanisms below 3V and explore synthesis techniques for lithium-rich materials (LRCMO).

The pristine LCMO was synthesized through a planetary milling process of the precursors, followed by a high-temperature calcination step. Overlithiation of LCMO was achieved through an additional step at medium-low temperature (200°C) under vacuum by mixing the pristine LCMO with LiI. Various chemical-physical characterization techniques were employed to evaluate the synthesis results. Specifically, ICP-OES quantified the additional lithium incorporated into the material chemically, while X-ray diffraction assessed the structural modifications that LCMO (originally with a cubic spinel structure) undergoes after overlithiation.

The synthesis of LCMO, initially reported by Eli et al. in 1998, involved varying the copper content in the $LiCuxMn_2\text{-}xO_4$ formula to optimize performance. This study extends that work by focusing on the lithiation mechanisms below 3V and studying the material also in full-cell configuration for the first time. Advanced electrochemical techniques, including cyclic voltammetry, galvanostatic charge-discharge tests, GITT, and EIS at different states of charge (SOC), were employed to investigate the lithiation mechanisms occurring in the material across various potential windows. Specifically, a mechanism of core-shell particle formation below 3V is proposed.

LCMO demonstrated a high working potential of around 5V due to the electrochemical activity of copper, which is beneficial for increasing the energy density of lithium-ion batteries. The material showed good cycle stability, maintaining capacity over multiple charge-discharge cycles. In particular, the lithium-rich material proved useful for stabilizing the performance of full-cell configurations due to the additional lithium content, which optimizes the cell formation phase and has positive effects on subsequent cycling phases by reducing the electrode potential slippage. The findings presented contribute to the broader understanding of high-voltage cathode materials and pave the way for developing more efficient and durable energy storage solutions.

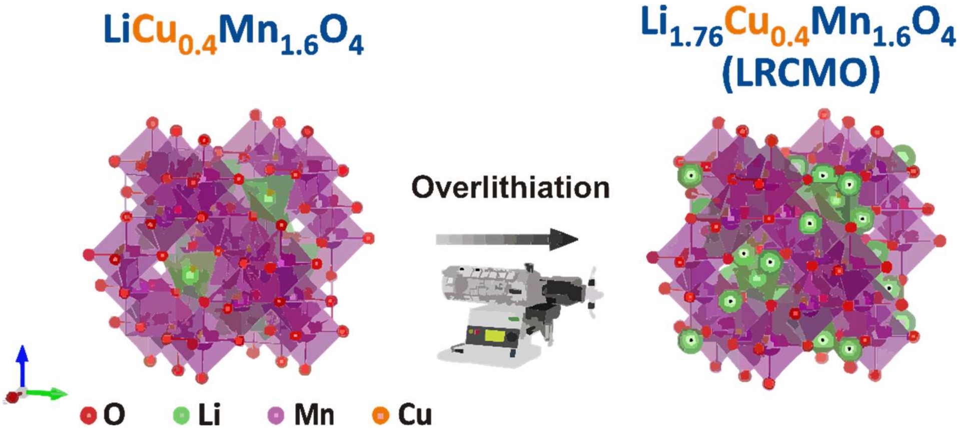

***Fig. 1:** Structure of LCMO and the over lithiated structure obtained after the chemical treatment with LiI.*

Key words: High voltage cathodes, lithium-ion batteries, Li-rich materials, Spinel oxide.

References

S. Mukerjee, J. T. Vaughey, J. Electrochem. Soc 1998, 145.

HYBRIDIZATION OF Li-ION AND SUPERCAPACITOR TECHNOLOGIES: PROMISING MÉLANGE

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YUNASKO-Ukraine LLC is the cutting-edge startup working in cooperation with the National Academy of Science of Ukraine on the development of supercapacitors (SCs) and their hybrids with Li-ion batteries. The latter can be called Li-ion Battery Intensified by Supercapacitor (LIBIS), and it differs from the known LIC technology since both positive and negative electrode (and also electrolyte) contain ingredients from LIB and SC technologies. We focus on low internal resistance because it can provide high power density with low heat generation and thus ensure safe operation. The highest efficiency of our SCs has been confirmed by a number of international experts, and the innovative LIBIS technology effectively combines the advantages of both "parents". Several sets of LIBIS pouch cells with their voltage of 2.7V and capacities from 1 Ah to 6 Ah have been manufactured at the YUNASKO pilot site. The second generation of LIBIS is currently at TRL3-4 level, exhibiting an energy density of 55-65 Wh/kg with the immediate goal of further increasing the energy density to 80-90 Wh/kg. The number of deep charge-discharge cycles of LIBIS exceeds 30K and they can be charged to 100% in 6 minutes.

Despite lower energy of YUNASKO hybrids compared to conventional Li-ion batteries, we can see new markets for this innovative technology in many applications with less critical requirements for the highest energy densities, while some other features such as fast charging, long service life, wide operating temperature range and safety are important. Some examples can be as follows:

- urban transport (taxi, delivery services, e-bikes and scooters, etc.) wherein long range is not as critical as the ability to charge quickly, a large number of charge-discharge cycles and elimination of thermal runaway during operation;
- smart grids in residential areas, in particular for frequency regulation and in combination with renewable energy sources;
- robotics and automated guided vehicles (AGV) for warehouses - currently they mainly use lead acid batteries and gradually moving to LiFePO4 (LFP) batteries (*NOTE*: issues with these technologies are similar: rather slow charging and short cycle life that does not enable to use such batteries for at least 3 years of operation required for robotics/AGV, with very frequent charging and discharging);
- various actuators in energy and industry sectors – both SCs and LIBIS can successfully replace some outdated mechanical systems, such as hydraulic or pneumatic;
- backup memory protection in data centers.

POSTER PRESENTATION

IMPACT OF VIBRATIONAL CONTRIBUTIONS ON THE EQUILIBRIUM VOLTAGE of *MOF*-LIKE ALKALI-Mn-*DOBDC* ELECTROCHEMICAL CELLS

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The equilibrium voltage of an electrochemical cell is calculated from Nernst equation as difference between Gibbs free energy in reduced / oxidized states. While the electronic structure component of the free energy is dominant, other contributions to total free energy cannot be ruled out. Our theoretical analysis indicates that vibrations can bring relatively important contributions for MOF-like systems of type alkali-Mn-DOBDC; remarkably, these contributions are significant for alkali=Na and K which allows us to check explicitly these results by comparing the voltages for Li2-, Na2-, K2- Mn-DOBDC. We found an unexpected increase of the cell voltage for Na an K cell compared to Li, which is typically not expected according to electrochemical potential data. Moreover, we show that the values of the vibrational corrections to calculated potential as difference of the vibrational free energy are comparable to experimental data, i.e. around 0.1-0.2 V.

Key words: DFT; MOF-electrodes; vibrations; free energy

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References

1. D. Rambabu, A.E. Lakraychi, J. Wang, L. Sieuw, D. Gupta, P. Apostol, G. Chanteux, T. Goossens, K. Robeyns, A. Vlad, An electrically conducting Li-ion metal–organic framework, *J. Am. Chem. Soc*. 143 (30) (2021) 11641–11650, http://dx.doi.org/10.1021/jacs.1c04591
2. C. Morari, L. Buimaga-Iarinca, C. Tripon, R.V.F. Turcu, Comparative study of the vibrational contributions to electrochemical potential in Na2 -Mn-DOBDC and Li2 -Mn-DOBDC electrodes, *Electrochimica Acta* 473 (2024) 143493, https://doi.org/10.1016/j.electacta.2023.143493

INNOVATIVE COORDINATION POLYMERS FOR POST-LITHIUM BATTERIES

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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 A4-PTtSA [3]. 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.

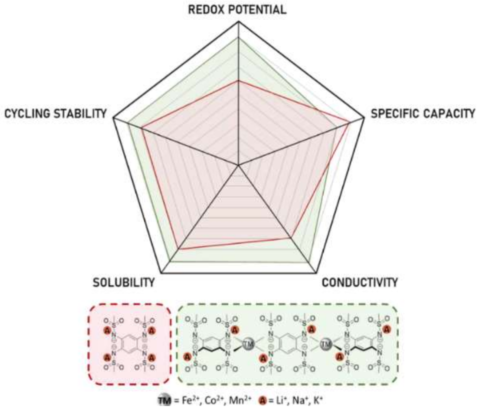

***Fig. 1:** Comparison of battery performance for A4-PTtSA and A2-TM-PTtSA organic cathode materials*

Key words: coordination polymer, conjugated sulfonamide, cathode material, post-Li batteries.

References

1. Ponrouch, Alexandre, et al., *Phil. Trans. R. Soc.*, 2019, 377, 20180297.
2. Wang, Jiande, et al., *Energy Environ. Sci.*, 2022, 15, 3923.
3. Wang, Jiande, et al., *ACS Energy Lett.*, 2022, 7, 668.

STRONG ION PAIRING AT THE ORIGIN OF MODIFIED Li-CATION SOLVATION AND IMPROVED PERFORMANCES OF DUAL-SALT ELECTROLYTES

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Organic phosphates have been widely used as fire-retardant additives and co-solvents to enhance the safety of Li-ion electrolytes. However, these solvents exhibit poor compatibility with low-potential electrodes and are ineffective as sole solvents at low salt concentrations. Although high-concentration electrolytes can improve interfacial properties by altering the solvation structure, they also suffer from low ionic conductivity, high viscosity, and increased costs.

In this study, we analyze a dual-salt phosphate-based electrolyte consisting of medium-concentration lithium nitrate ($LiNO_3$) and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) salts in triethyl phosphate (TEP). This formulation addresses the issues mentioned above. The strong affinity between NO_3 and Li^+ allows Li NO_3 to disrupt the solvation structure, with mixed anion (NO_3 and TFSI) pairing with Li^+. The environment of Li^+ in the dual-salt phosphate-based electrolyte is examined using nuclear magnetic resonance and Raman analysis, supported by theoretical calculations [1].

The findings indicate that the dual-salt formulation leads to the formation of a $LiF\text{-}Li_3N\text{-}LiN_xO_y$-rich solid-electrolyte interphase on the Li metal surface. These results not only enable the assembly of $LiNi_{0.5}Co0.2Mn_{0.3}O_2$||Li cells with significantly improved cycling and low-temperature performance but also provide insights into managing strong polarity phosphate electrolytes through fine solvation interplay.

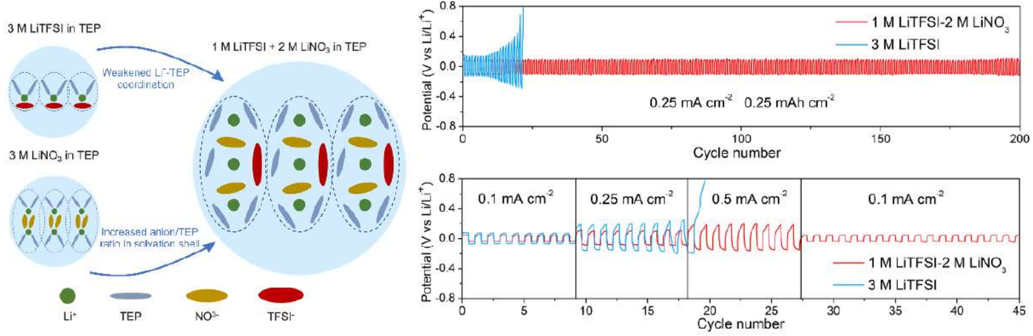

***Fig. 1:** Benefiting from the strong affinity of NO3− towards Li+, an unusual solvation structure is attained in organic phosphate solvent electrolyte, which leads to the formation of LiF-LiNxOy-rich solid-electrolyte interphase (SEI) on Li metal, with thus reversible and long-term Li electrodeposition-electro dissolution attained*

Key words: Li-metal batteries, dual-salt electrolyte, solvation structure, ion pairing, solid-electrolyte interphase

References

1. X. Zhang *et al.*, "Strong ion pairing at the origin of modified Li-cation solvation and improved performances of dual-salt electrolytes," *J. Power Sources*, vol. 541, no. February, p. 231644, 2022, doi: 10.1016/j.jpowsour.2022.231644.

BIMETALLIC ANIONIC ORGANIC FRAMEWORKS WITH SOLID-STATE CATION CONDUCTION FOR CHARGE STORAGE APPLICATIONS

Yan Zhang, Jiande Wang, Petru Apostol, Darsi Rambabu, Alae Eddine Lakraychi, Xiaolong Guo, Xiaozhe Zhang, Xiaodong Lin, Shubhadeep Pal, Vasudeva Rao Bakuru, Xiaohua Chen, Alexandru Vlad*

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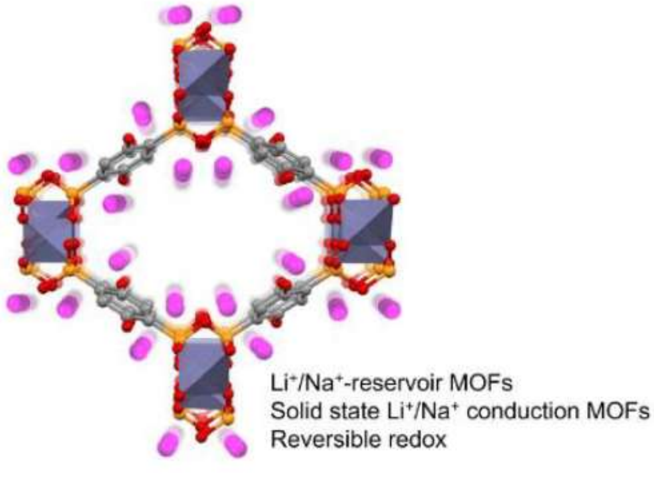
A new phosphonate-based anionic bimetallic organic framework, with the general formula of A_4-Zn-DOBDP (wherein A is Li^+ or Na^+, and $DOBDP^{6-}$ is the 2,5-dioxido-1,4-benzenediphosphate ligand) is prepared and characterized for energy storage applications. With four alkali cations per formula unit, the A_4-Zn-DOBDP MOF is found to be the first example of non-solvated cation conducting MOF with measured conductivities of 5.4 × 10-8 S cm^{-1} and 3.4×10^{-8} S cm^{-1} for Li^{4-} and Na^{4-} phases, indicating phase and composition effects of Li^+ and Na+ shuttling through the channels. Three orders of magnitude increase in ionic conductivity is further attained upon solvation with propylene carbonate, placing this system among the best MOF ionic conductors at room temperature. As positive electrode material, Li_4-Zn-DOBDP delivers a specific capacity of 140 mAh g^{-1} at a high average discharge potential of 3.2 V (vs. Li^+/Li) with 90% of capacity retention over 100 cycles. The significance of this research extends from the development of a new family of electroactive phosphonate-based MOFs with inherent ionic conductivity and reversible cation storage, to providing elementary insights into the development of highly sought yet still evasive MOFs with mixed-ion and electron conduction for energy storage applications.



Key words: *Metal-organic framework; Organic battery; Solid-state ionic conduction; High voltage; Alkali ion storage.*

Acknowledgments *(if applicable)*

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References

Zhang, Y et al., *Angew. Chem. Int. Ed.,* 2023, 202310033.

AN ELECTRICALLY CONDUCTING ALKALI-ION METAL–ORGANIC FRAMEWORK CATHODES

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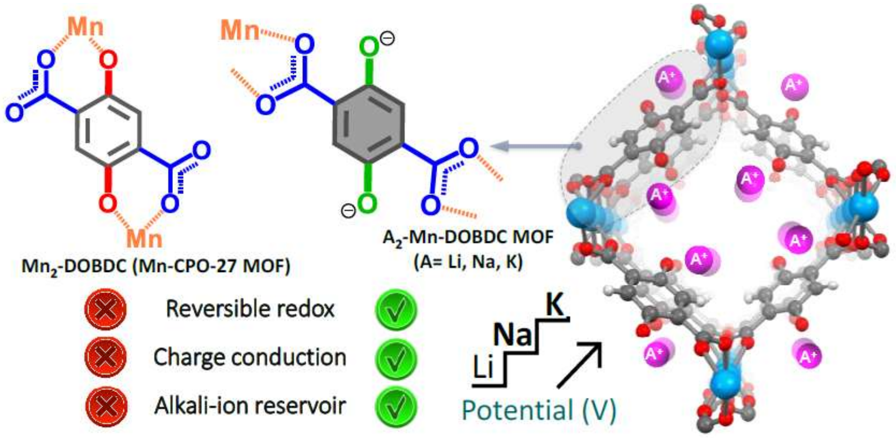
Metal–organic frameworks (MOFs) have emerged as an important, yet highly challenging class of electrochemical energy storage materials. The chemical principles for electroactive MOFs remain, however, poorly explored because precise chemical and structural control is mandatory. Herein, we present on electrically 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. The accurate chemical and structural changes not only enable reversible redox but also induce a million-fold electrical conductivity increase by virtue of efficient electronic self-exchange facilitated by mix-in redox: 10^{-7} S/cm for Li_2-Mn-DOBDC vs 10^{-13} S/cm for the isoreticular Li_2-Mg-DOBDC, or the Mn-CPO-27 compositional analogues. This particular SBU topology also considerably augments the redox potential of the $DOBDC^{4-}$ linker (from 2.4 V up to 3.2 V, vs Li^+/Li^0), a highly practical feature for Li-ion battery assembly and energy evaluation [1]. Further investigation of Li_2-Mn-DOBDC into Na and K versions is currently ongoing. It has been observed that the potential order reverses, with Li < Na < K, due to vibrational energy changes influenced by the size of the cations [2].



Key words: Electrical conductivity, cathodes Metal-organic frameworks, Redox reactions

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References

1. Rambabu, D.; Lakraychi, A.E; Wang, J.; Sieuw, L.; Gupta, D.; Apostol, P.; Chanteux, G.; Goossens, T.; Robeyns, K.; and Vlad, A. *J. Am. Chem. Soc. 2021*, 143, 30, 11641–11650.
2. Morari, C.; Buimaga-Iarinca, L.; Tripon C.; Turcu, R.V.F. *Electrochim. Acta,* 2024, 473, 143493.

REVEALING THE REVERSIBLE SOLID-STATE ELECTROCHEMISTRY OF LITHIUM-CONTAINING CONJUGATED OXIMATES: TOWARDS A NEW FUNCTIONALITY FOR ORGANIC BATTERIES

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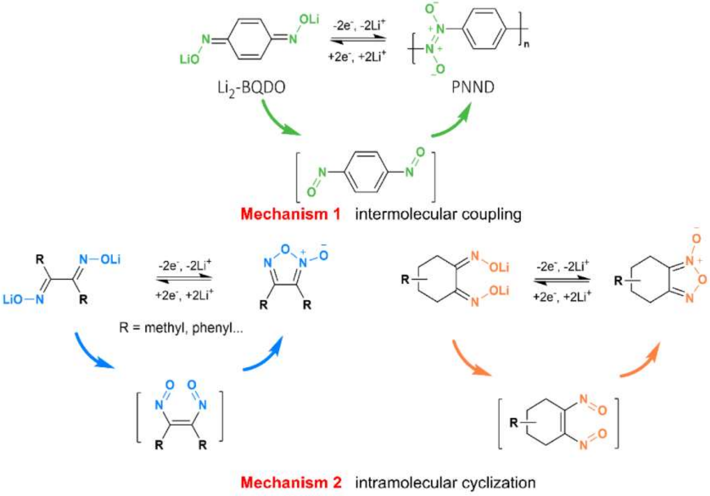
In the rising advent of organic Li-ion positive electrode materials with increased energy content, chemistries with high redox potential and intrinsic oxidation stability remain a challenge. Herein, we report the solid-phase reversible electrochemistry of the oximate organic redox functionality. The 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.



Key words: conjugated oximates, functionality, Organic batteries

Acknowledgments
Author acknowledges to ERC, and FSR-FNRS.

References

1. Wang, J., Apostol, P., Rambabu, D., Guo, X., Liu, X., Robeyns, K., Du, M., Zhang, Y., Pal, S., Markowski, R., Lucaccioni, F., Lakraychi, A.E, Morari, C., Gohy, J-F., Gupta, D., Vlad, A. *Sci. Adv*., 2023, eadg6079.

TOWARDS THE 4V-CLASS N-TYPE ORGANIC LITHIUM-ION POSITIVE ELECTRODE MATERIALS: THE CASE OF CONJUGATED TRIFLIMIDES AND CYANAMIDES

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Organic electrode materials have garnered a great deal of interest owing to their sustainability, cost-efficiency, and design flexibility metrics. Despite numerous endeavors to fine-tune their redox potential, the pool of organic positive electrode materials with a redox potential above 3 V *versus* Li^+/Li^0, and maintaining air stability in the Li-reservoir configuration remains limited. This study expands the chemical landscape of organic Li-ion positive electrode chemistries towards the 4 V-class through molecular design based on electron density depletion within the redox center *via* the mesomeric effect of electron-withdrawing groups (EWGs). This results in the development of novel families of conjugated triflimides and cyanamides as high-voltage electrode materials for organic lithium-ion batteries. These are found to exhibit ambient air stability and demonstrate reversible electrochemistry with redox potentials spanning the range of 3.1 V to 3.8 V (*versus* Li^+/Li^0), marking the highest reported values so far within the realm of n-type organic chemistries Fig. 1. Through comprehensive structural analysis and extensive electrochemical studies, we elucidate the relationship between the molecular structure and the ability to fine-tune the redox potential. These findings offer promising opportunities to customize the redox properties of organic electrodes, bridging the gap with their inorganic counterparts for application in sustainable and eco-friendly electrochemical energy storage devices [1].

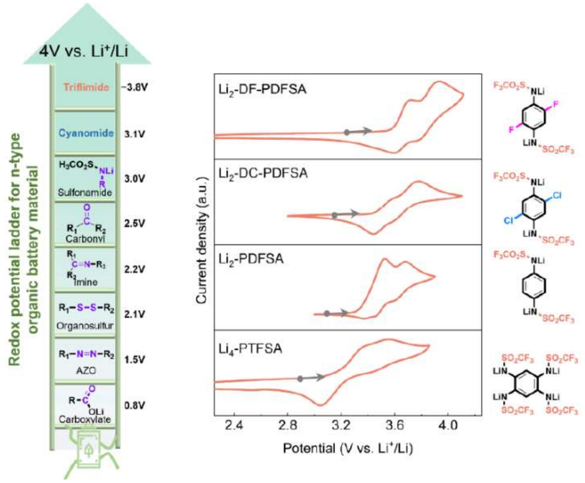

Fig. 1: *The redox potential ladder for n-type organic battery materials and the cyclic voltammetry of triflimides.*

Key words: high-voltage electrode materials, electron-withdrawing groups, triflimides, cyanamides.

References

1. X. Guo, P. Apostol, X. Zhou, J. Wang, X. Lin, D. Rambabu, M. Du, S. Er, A. Vlad, *Energy Environ. Sci*. 2023, 17, 173.

EXPLORING CHARGE TRANSPORT AND ELECTROCHEMICAL CAPACITANCE IN 2D CONDUCTIVE MOFs: EFFECTS OF NITROGEN-RICH LIGANDS AND INTERLAYER SPACING

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Two-dimensional electrically conducting metal–organic frameworks (2D-e-MOFs) are highly promising for various applications, including energy storage in electrochemical capacitors (ECs). Despite advances, developing systems that allow post-synthetic chemical functionalization and fine-tuning of transport properties remains challenging. We present two isostructural 2D-e-MOFs: $Ni_3(HIH_3\text{-}TAT)_2$ and $Ni_3(HITBim)_2$, based on 2,3,7,8,12,13-hexaaminotriazatruxene (HATAT) and 2,3,8,9,14,15-hexaaminotribenzimidazole (HATBim). These frameworks exhibit temperature-activated charge transport with conductivity values of 44 and 0.5 mS cm^{-1}, respectively. Density functional theory analysis attributes this difference to variations in electron density distribution within the ligands, with nitrogen-rich HATBim showing more localized electron density and a lower LUMO energy. Post functionalization with methanesulfonyl groups on $Ni_3(HITAT)_2$ modulates its electrical conductivity by a factor of ∼20, offering a design blueprint for tunable functional materials1. Additionally, we investigated the charge storage mechanisms of triazatruxene-based 2D MOFs with variable alkyl groups: $Ni_3(HIR_3\text{-}TAT)_2$ (R=H, Et, n-Bu, n-Pent). Alkyl groups modulate interlayer spacing, shifting the charge storage mechanism from double-layer capacitance to pseudo capacitance, enhancing molar specific capacitance from $Ni_3(HIH_3\text{-}TAT)_2$ to $Ni_3(HIBu_3\text{-}TAT)_2$. Partial exfoliation of $Ni_3(HIBu_3\text{-}TAT)_2$ increases accessibility of redox-active sites, enhancing faradaic processes. This strategy may guide the design of advanced electrode materials for ECs[2].

Key words: conducting MOFs, post-synthetic chemical functionalization, charge storage, specific capacitance.

References

1. Apostol, P.; Gali, S. M.; Su, A.; Tie, D.; Zhang, Y.; Pal, S.; Lin, X.; Bakuru, V. R.; Rambabu, D.; Beljonne, D.; Dincă, M.; Vlad, A. *J. Am. Chem. Soc*. 2023, 145, 24669-24677
2. A. Y. Su, P. Apostol, J. Wang, A. Vlad, M. Dincă, *Angew. Chem. Int. Ed*. 2024, 63, e202402526.

DICARBONATE SOLVENT ELECTROLYTE FOR HIGH PERFORMANCE 5 V-CLASS LITHIUM-BASED BATTERIES

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Rechargeable lithium batteries using 5 V positive electrode materials can deliver considerably higher energy density as compared to state-of-the-art lithium-ion batteries [1]. However, their development remains plagued by the lack of electrolytes with concurrent anodic stability and Li metal compatibility [2]. Here we report a new electrolyte based on dimethyl 2,5-dioxahexanedioate solvent for 5 V-class batteries [3]. Benefiting from the particular chemical structure, weak interaction with lithium cation and resultant peculiar solvation structure, the resulting electrolyte not only enables stable, dendrite-free lithium plating-stripping, but also displays anodic stability up to 5.2 V (vs. Li/Li+), in additive or co-solvent-free formulation, and at low salt concentration of 1 M. Consequently, the Li || $LiNi_{0.5}Mn_{1.5}O_4$ cells using the 1 M $LiPF_6$ in 2,5-dioxahexanedioate based electrolyte retain >97% of the initial capacity after 250 cycles (Fig. 1), outperforming the conventional carbonate-based electrolyte formulations, making this, and potentially other dicarbonate solvents promising for future Lithium-based battery practical explorations.

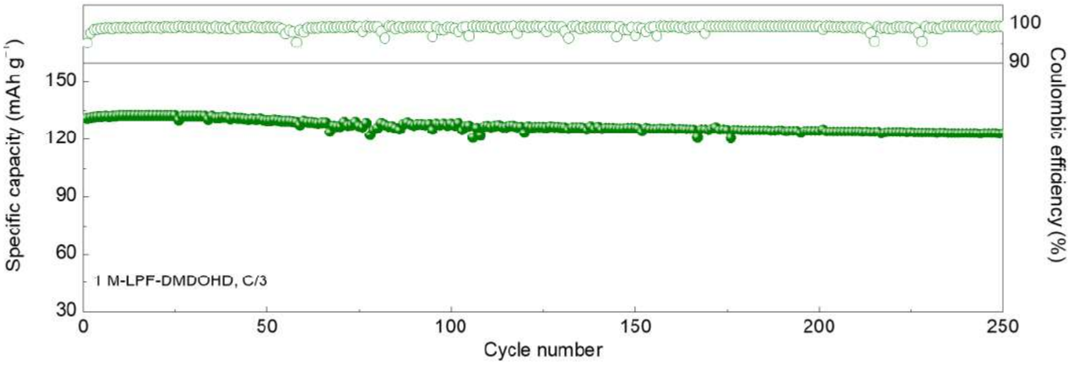

Fig. 1: *Cycling stability of the Li||$LiNi_{0.5}Mn_{1.5}O_4$ cell with 1 M $LiPF_6$ in dimethyl 2,5-dioxahexanedioate (1 M-LPF-DMDOHD) electrolyte cycled at rate of C/3.*

Key words: Lithium metal battery; 5 V-class cathode material; dicarbonate electrolyte solvent; dimethyl 2,5-dioxahexanedioate; dendrite-free lithium plating/stripping; carbonate-based electrolyte

Acknowledgments

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References

1. Zhang, Z.; Hu, L.; Wu, H.; Weng, W.; Koh, M.; Redfern, P.; Curtiss, L.; Amine, K. *Energy Environ. Sci.*, 2013, *6* 1806.
2. Fan, X.; Chen, L.; Borodin, O.; Ji, X.; Chen, J.; Hou, S.; Deng, T.; Zheng, J.; Yang, C.; Liou, S.; Amine, K.; Xu, K.; Wang, C. *Nat. Nanotechnol.*, 2018, *13*, 715.
3. Zhang, X.; Xu, P.; Duan, J.; Lin, X.; Sun, J.; Shi, W.; Xu, H.; Dou, W.; Zheng, Q.; Yuan, R.; Wang, J.; Zhang, Y.; Yu, S.; Chen, Z.; Zheng, M.; Gohy, J.; Dong, Q.; Vlad, A. *Nat. Commun.*, 2024, *15*, 536.

DESIGN PRINCIPLES OF QUINONE REDOX SYSTEMS FOR ADVANCED SULFIDE SOLID-STATE ORGANIC LITHIUM METAL BATTERIES

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The emergence of solid-state battery technology presents a potential solution to the dissolution challenges of high-capacity small molecule quinone redox systems [1]. Nonetheless, the successful integration of argyrodite-type Li_6PS_5Cl, the most promising solid-state electrolyte system, and quinone redox systems remains elusive due to their inherent reactivity [2]. Here, a library of quinone derivatives is selected as model electrode materials to ascertain the critical descriptors governing the (electro)chemical compatibility and subsequently the performances of Li_6PS_5Cl-based solid-state organic lithium metal batteries (LMBs) [3]. Compatibility is attained if the lowest unoccupied molecular orbital level of the quinone derivative is sufficiently higher than the highest occupied molecular orbital level of Li_6PS_5Cl. The energy difference is demonstrated to be critical in ensuring chemical compatibility during composite electrode preparation and enable high-efficiency operation of solid-state organic LMBs. Considering these findings, a general principle is proposed for the selection of quinone derivatives to be integrated with Li_6PS_5Cl, and two solid-state organic LMBs, based on 2,5-diamino-1,4-benzoquinone and 2,3,5,6-tetraamino-1,4-benzoquinone, are successfully developed and tested for the first time. Validating critical factors for the design of organic battery electrode materials is expected to pave the way for advancing the development of high-efficiency and long cycle life solid-state organic batteries based on sulfides electrolytes.

Key words: lithium organic batteries; organic cathodes; solid-state lithium metal batteries; sulfide electrolytes

Acknowledgments
The authors acknowledge F.R.S.-FNRS, ERC, and Marie Skłodowska-Curie Actions for financial support.

References

1. Hao, F.; Chi, X.; Liang, Y.; Zhang, Y.; Xu, R.; Guo, H.; Terlier, T.; Dong, H; Zhao, K.; Lou, J.; Yao, Y. *Joule*, 2019, *3* 1349.
2. Ji, W.; Zhang, X.; Xin, L.; Luedtke, A.; Zheng, D.; Huang, H.; Lambert, T.; Qu, D. *Energy Storage Mater.*, 2022, *45*, 680.
3. Lin, X.; Apostol, P.; Xu, H.; Bakuru, V.; Guo, X.; Chen, Z.; Rambabu, D.; Pal, S.; Tie, D.; Zhang, Y.; Xie, X.; Kim, S.; Li, Y.; Li, Z.; Du, M.; Yuan, R.; Zheng, M.; Gauthy, F.; Finsy, V.; Zou, J.; Gohy, J.; Dong, Q.; Vlad, A. *Adv. Mater.*, 2024, 2312908. https://doi.org/10.1002/adma.202312908.

DIRECT NON-SACRIFICIAL ELECTROSYNTHESIS OF $Ni_3(HITP)_2$ NANOSTRUCTURES FOR MICRO-SUPERCAPACITOR INTEGRATION

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Micro-supercapacitors are emerging as an important electrical energy storage technology expected to play a critical role in the large-scale deployment of autonomous microdevices for health, sensing, monitoring, and other IoT applications. Electrochemical double-layer capacitive storage requires a combination of high surface area and high electronic conductivity, with these being attained only in porous or nanostructured carbons. However, techniques for conformal deposition at micro- and nano-scale of these materials are complex, costly, and hard to upscale. [1, 2] Recently, conducting metal organic frameworks (MOFs) appeared as extraordinary candidates to cope the challenges, with techniques accessible to provide thin large area film materials. [3]
Herein, we present the direct, one step non-sacrificial anodic electrochemical deposition of Ni_3(2,3,6,7,10,11-hexaiminotriphenylene)$_2$ - $Ni_3(HITP)_2$, a porous and electrically conducting MOF (**Fig. 1**). Employing this strategy enables the growth of $Ni_3(HITP)_2$ films on a variety of 2D substrates as well as on 3D nanostructured substrates to form $Ni_3(HITP)_2$ nanotubes and Pt@$Ni_3(HITP)_2$ core-shell nanowires. Based on the optimal electrodeposition protocols, Ni3(HITP)2 films interdigitated micro-supercapacitors are fabricated and tested as a proof of concept, attesting the convincing efficiency of the deposition method. [4]

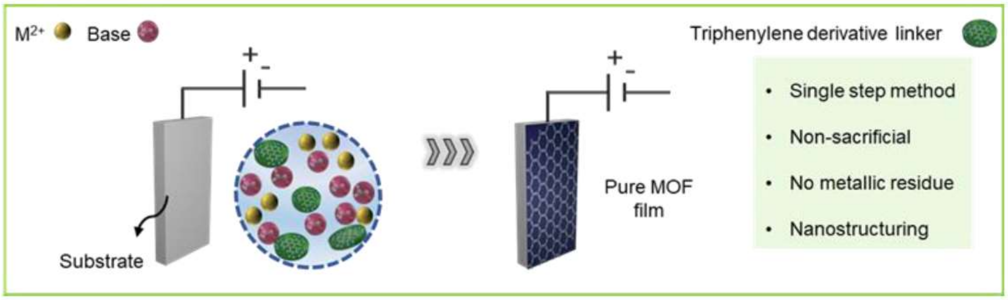

***Fig. 1:** Schematics of the electrodeposition strategy of $Ni_3(HITP)_2$ including the main benefits of our method.*

Key words: one-step anodic electrodeposition, conductive metal-organic frameworks, 3D nanostructures, interdigitated micro supercapacitors.

References:

1. Zhang, X.; Wan, K.; Subramanian, P.; Xu, M.; Luo, J.; Fransaer, J., *J. Mater. Chem. A 2020*, *8*(16), 7569-7587.
2. Mu, X., Wang, W., Sun, C., Wang, J., Wang, C., & Knez, M., *Advanced Materials Interfaces* 2021, *8*(9), 2002151.
3. Sheberla, D., Bachman, J. C., Elias, J. S., Sun, C. J., Shao-Horn, Y., & Dincă, M., *Nat. Mater.* 2017, *16*(2), 220-224.
4. Behboudikhiavi, S., Chanteux, G., Babu, B., Faniel, S., Marlec, F., Robert, K., … & Vlad, A., *Small* 2024, 2401509.

OPTIMIZATION OF WATERBORNE CATHODE PRODUCTION FOR LITHIUM-ION BATTERIES: INVESTIGATING BINDERS, CURRENT COLLECTORS, AND CALENDERING EFFECTS

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Lithium-ion batteries (LIBs) are pivotal in the global transition toward sustainable energy solutions, crucial for the automotive industry's shift to electric vehicles (EVs), and vital components in energy storage systems. The increasing demand for efficient, high-performance LIBs necessitates innovative approaches to cathode production. This study focuses on developing cathodes using a waterborne pathway, transitioning from lab-scale production to a small pilot line. Central to this work is the use of Lithium Nickel Manganese Oxide (LNMO) as the active material, exploring the influence of three critical factors: binder selection, current collector type, and the application of a calendering process. Two types of binders, analogous to commercially available polymeric binders such as Styrene-Butadiene Rubber (SBR), are used in conjunction with Carboxymethyl Cellulose (CMC). The study compares pristine battery-grade aluminum foil with carbon-coated aluminum foil as current collectors. Additionally, the effect of a calendering step post-electrode production is assessed to understand its impact on electrochemical performance.

The research employs various combinations of these variables. Comprehensive analyses are conducted using Field Emission Scanning Electron Microscopy (FESEM), galvanostatic cycling, and Potentiostatic Electrochemical Impedance Spectroscopy (PEIS). Preliminary results indicate that the current collector coating significantly affects electrode performance, while the role of calendering remains under investigation.

This study offers crucial insights into optimizing waterborne cathode production processes, potentially enhancing the scalability and performance of lithium-ion batteries. Such advancements are vital for supporting the green transition in the automotive sector and broader applications of LIBs in energy storage systems.

Key words: LNMO, waterborne cathode production, process optimization

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TIN-BASED ANODES FOR SODIUM ION BATTERIES

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Tin-based compounds represent promising anodes materials for sodium ion batteries (SIBs) due to their high capacity compared to traditional insertion-based anodes. A significant hurdle in their application lies in the large volume changes experienced by metallic tin electrodes during sodiation, leading to electrode pulverization. Extensive research has delved into understanding and mitigating this challenge, focusing particularly on controlling cracking, managing solid electrolyte interface (SEI) formation and engineering electrodes with different microstructures to prevent rapid capacity degradation.

Electrolyte additives, like fluoroethylene carbonate, and functional binders such as polyacrylate are proposed to play a crucial role in enhancing capacity retention by promoting a passivation film and mitigating the effects of volume changes [1, 2]. This work investigates the impact of binders and electrolytes on tin nanoparticle anodes using electrochemical methods. Charge-discharge cycling, and cyclic voltammetry will be complemented by ex situ analyses including scanning electron microscopy and X-ray diffraction to provide insights into reactions reversibility, structural integrity, and binder-electrode adhesion morphology.

Furthermore, the optimal cut-off voltage will be explored to enhance reaction reversibility and promote the formation of a compact SEI layer. The chemical composition, resistance and capacitance of the SEI layer will offer valuable insights into its formation and stability, crucial for improving stability and reversibility of tin anodes. The findings underscore the importance of electrolyte and binder selection in improving the stability and overall performance of tin-based anodes, offering insights crucial for advancing battery technologies.

Key words: Tin-based anodes, Sodium ion batteries, Electrolyte interface, Degradation.

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References

1. Fukunishi, M., Yabuuchi, N., Dahbi, M., Son, J.Y., Cui, Y., Oji, H. and Komaba, S., 2016. Impact of the cut-off voltage on cyclability and passive interphase of Sn-polyacrylate composite electrodes for sodium-ion batteries. *The Journal of Physical Chemistry C*, 120(28), pp.15017-15026.
2. Komaba, S., Matsuura, Y., Ishikawa, T., Yabuuchi, N., Murata, W. and Kuze, S., 2012. Redox reaction of Sn-polyacrylate electrodes in aprotic Na cell. *Electrochemistry Communications*, 21, pp.65-68.

COVALENT ORGANIC FRAMEWORK ELECTRODE MATERIALS FOR Li-ION BATTERIES

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Lithium-ion batteries (LIBs) are considered highly promising for storing electrochemical energy from renewable sources and for enabling long-range electric vehicles. However, the growing demand for certain key raw materials used in LIBs (lithium, cobalt, etc.) could lead to supply issues in the near future and raise significant environmental concerns. As a result, organic electrode materials have garnered considerable attention as an alternative to inorganic electrodes. [1] Covalent organic frameworks (COFs) are crystalline porous organic polymers that have emerged as promising organic electrodes for LIBs due to their insolubility in electrolyte, the possibility to introduce numerous redoxactive sites and tuneable porosity to facilitate ion diffusion. [2] A more detailed study must be undertaken to improve the capacity and conductivity of these materials. My project is focused on the
synthesis of new 2D electroactive COF to be used as organic cathodes in lithium-ion batteries and in improving their electrochemical performance by processing such materials.

Key words: Covalent Organic Framework, organic batteries, electroactive porous materials.

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References

1. Y. Lu, J. Chen, Nat. Rev. Chem. 2020, 4, 127-142.
2. R. Dantas, C. Ribeiro, M. Souto. Chem. Commun. 2024, 60, 138-149.

ELECTRODEPOSITION OF LITHIUM METAL: A NOVEL APPROACH USING ORGANIC SOLVENTS AND IONIC LIQUIDS

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For a range of applications, particularly in battery technology, there is a growing need for uniform, high-quality metallic lithium, or lithium-coated materials. However, electrodeposition techniques have not been practical or cost-effective due to the low solubility of most lithium salts in suitable solvents. This study proposes efficient lithium electrodeposition processes and electrolyte baths that can be operated at low temperatures and with relatively low costs. The electrolyte used was a mixture of dimethyl sulfoxide (DMSO) and the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate (BMIMPF6), with lithium nitrate ($LiNO_3$) as the lithium source. Lithium metal was deposited onto copper substrates at room temperature at selected current densities within an argon-filled glovebox, using either a power source or a PARSTAT-4000A potentiostat. The deposition process was characterized by cyclic voltammetry (CV) and Fourier-transform infrared spectroscopy (FTIR). The resulting deposits were analysed by visual inspection, scanning electron microscopy (SEM) and X-ray diffraction (XRD). XRD analysis confirmed the presence of lithium, as well as occasional lithium hydroxide or lithium oxide. However, the adhesion of the lithium to the copper substrate was poor when large amounts were deposited, leading to irregular detachment of the lithium into the electrolyte.

Fig. 1: *The obtained deposit after 5h at 5.25V, 0.01A*

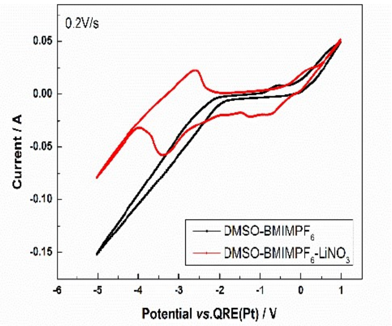

Fig. 2: *Cyclic voltammograms of the electrolyte for Li electrodeposition and of the background*

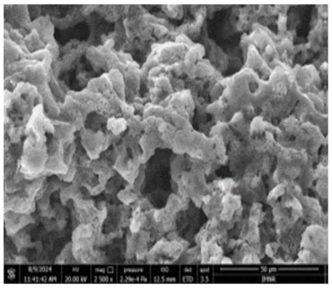

Fig. 3: *SEM image of the Li deposit on Cu foil, with X2500 magnification*

Key words: lithium electrodeposition, organic/ionic liquids solvents, X-ray diffraction, scanning electron microscopy, Fourier-transform infrared spectroscopy, cyclic voltammetry.

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UNDERSTANDING THE INFLUENCE OF MECHANOCHEMICAL SYNTHESIS OF Li_3InCl_6 HALIDE SOLID ELECTROLYTE

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Climate change and a steady supply of sustainable energy are the global challenges arising today. As the world is changing over to electric modes of transportation in hopes of reducing carbon emissions, their backbone, battery technologies, has become a hot topic of development. Although Li-ion battery technology is currently the best-performing technology for energy storage sectors, it suffers from the sensitivity of catching fire due to liquid organic electrolytes. [1] The uptake of portable devices and electric vehicles is expected to go together with the availability of Solid-state Li-ion batteries (SSBs) with safety-improving solid electrolytes (SEs). They have several benefits compared to conventional LIBs: cost, performance, safety, thermal stability, and sustainability. Most recently, halide-based solid electrolyte (HSE) materials have emerged as potential inorganic electrolytes for SSB thanks to their moderate-high ionic conductivity at room temperature and their high-voltage wide electrochemical stability (compatible with 4V cathode materials) compared to other SEs such as polymers, oxides, or sulfides. [2,3] The synthesis of HSE materials requires moderate temperatures for the material preparation, high ductility, and easy densification steps in full-cell manufacturing. [4] Still, there is more understanding between the ionic transport and the Li/HSE interface dynamics is essential to optimize halide-based SSB. In this work, we report the advantages and potential of Li_3InCl_3 (LIC) halide as a solid-state electrolyte. First, we proposed solid-state synthesis via the mechanochemical method (ball-milling approach) with different milling time ranges from 8h to 40h. Utilizing two different milling environmental conditions, argon condition ball milled samples and dry air induced dry room condition ball milling samples. Using various characterization tools such as X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Electrochemical Impedance Spectroscopy (EIS) to understand the structural changes, morphology influences, and ionic transport mechanism during the different milling times. From the dry room ball milling approach, LIC presents a high ionic conductivity of around 0.4 $mS.cm^{-1}$, compared to argon gas condition ball milled samples of 0.2 $mS.cm^{-1}$ at room temperature. Overall, this approach provides insights about the milling time, milling conditions, and influence of particle size, which is more important for future upscaling HSEs and LIC as a promising candidate for use as electrolyte Li-metal-based SSB.

Key words: halide solid electrolytes, ball-milling method, Li3InCl6, solid-state battery, material design

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References

1. H. Cavers, P. Molaiyan, M. Abdollahifar, U. Lassi, A. Kwade, Perspectives on Improving the Safety and Sustainability of High Voltage Lithium-Ion Batteries Through the Electrolyte and Separator Region, *Adv. Energy Mater*. 12 (2022) 2200147. https://doi.org/https://doi.org/10.1002/aenm.202200147.
2. A. Manthiram, X. Yu, S. Wang, Lithium battery chemistries enabled by solid-state electrolytes, *Nat. Rev. Mater.* 2 (2017) 16103. https://doi.org/10.1038/natrevmats.2016.103.
3. J. Janek, W.G. Zeier, Challenges in speeding up solid-state battery development, *Nat. Energy* 8 (2023) 230–240. https://doi.org/10.1038/s41560-023-01208-9.
4. Q. Wang, Y. Zhou, X. Wang, H. Guo, S. Gong, Z. Yao, F. Wu, J. Wang, S. Ganapathy, X. Bai, B. Li, C. Zhao, J. Janek, M. Wagemaker, Designing lithium halide solid electrolytes, *Nat. Commun*. 15 (2024) 1050. https://doi.org/10.1038/s41467-024-45258-3.

$LiNi_{0.5}Mn_{1.5}O_4$ EVOLUTION UPON AMBIENT CONDITIONS

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Since the surface plays an important role in the electrochemical performance of $LiNi_{0.5}Mn_{1.5}O_4$(LNMO) cathode materials, surface analysis and evolution can be helpful to understand the electrochemical behavior upon aging. For instance, ambient storage analyses is useful to determine how this material should be stored for long periods of time, or how the storage conditions can affect the surface structure and chemistry, and consequently, the electrochemical performances.

We study and compare the evolution of surface chemistry, bulk crystal structure and elemental content evolution and distribution of LNMO using a variety of characterization techniques including STEM-EDS-EELS, as well as electrochemical analysis.

Key words: LNMO, cathode, surface, storage conditions, aging.

DESIGNING Bi-METALLIC PHENANTHROLINE-BASED MOFs TOWARDS CHARGE TRANSPORT ELUCIDATION FOR ENERGY STORAGE APPLICATIONS

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Conductivity in Metal Organic Frameworks has long remained a mystery for researchers. Since 2009, diverse conductive MOFs (c-MOFs) families were designed, and provide smart tools to tune electrical conductivity, which can be uniquely combined with the intrinsic porosity of such materials [1,2]. Herein, we propose the design of a new family of bimetallic MOFs based on 1,10-phenanthroline-5,6-dione ligand bonded with different combinations of metal cations [3,4]. First extended with Cl-, Br- anions and Li+ cation using supramolecular interactions [5], the MOF systems extended by various Mn+ cations are expected to demonstrate electrical conductivity properties via through-bond transport due to the long-range conjugation of the resulting framework. This work aims at deepening the understanding of charge transport in MOFs and the tunability of different metal cations combinations. Furthermore, the transport properties and mechanisms are studied to evaluation the future possibilities for utilization as energy storage materials.

Key words: Metal organic Framework, self-assembly, electrical conductivity, ion conduction

References:

1. Xie, L., Skorupskii, G. & Dincă, M., *Chem. Rev.,* 2020, 120, 8536.
2. Lehn, J.-M., Supramolecular chemistry. *Concepts and perspectives*, 1995, New York: Vch, Weinheim.
3. Calucci, L., ..., Prescimone, A., *Inorg. Chim. Acta*, 2006, 359, 3911.
4. Gupta, D., Lakraychi, A. E., ..., Volder, M. D., Vlad, A., *Chem. Euro. J.*, 2022, e202201220.
5. Gupta, D., Chanteux, G., Kumar, G., Robeyns, K., and Vlad, A, *Chem. Sci.*, 2023, 14, 36, 9780-9786.

GRAPHENE MIXED WITH POLYIMIDE RESIN AS A PROTECTIVE LAYER TO MODIFY ZINC ANODE TO IMPROVE THE CYCLING STABILITY OF ZINC ION CAPACITORS

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The high energy density of the battery and the high power density of the supercapacitor are combined to form a new energy storage system—Metal ion hybrid supercapacitors. Among them, Zinc ion capacitors (ZICs) has become the most promising energy storage device due to higher power density and energy density. Similarly, ZICs also have shortcomings that exist in batteries, such as short circuits caused by zinc dendrites, poor cycling performance, etc. In this work, ZIC was assembled with YP-50 carbon materials as cathode, zinc foil as anode and 3 M zinc sulfate as electrolyte. In addition, we used graphene and polyimide resin to prepare a zinc anode protective layer, and compared the performance with bare zinc-based ZIC. The protective layer of graphene and polyimide resin not only guides zinc ions to uniformly plate on the zinc anode and reduces the formation of zinc dendrites, but also reduces the corrosion of the zinc anode, thereby improving the coulombic efficiency and cycle performance of ZIC.

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References

1. A. Xia *et al.*, Appl. Surf. Sci. 481 (2019) 852-859.
2. L. Kang *et al.*, Adv. Energy Mater. (2018) 1801090.

CURRENT TRENDS IN *SOFC* RESEARCH AND DEVELOPMENT

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The SOFC market is projected to grow significantly, reaching a market size of $6.8 billion by 2033. Key applications driving growth include transportation, military, data centers, and residential combined heat and power (CHP) [1], Japan and South Korea possessing the largest SOFC market.
The latest advancements in SOFC materials focus on developing new electrolytes, anodes and cathodes with improved ionic conductivity, fuel flexibility, and catalytic activity, especially for low and intermediate temperature operation. Materials with different crystalline structures, compositions, and morphologies have been synthesized and investigated for the SOFC components. Moreover, novel fabrication techniques like infiltration and thin-film deposition are enabling the use of a wider range of materials to optimize SOFC performance and durability [2].

Key words: solid oxides; nanostructures; sol-gel; electrical properties; thermal behaviour.

References

1. Affandi, N.S.M., Osman, N., *Materials Today Proceedings* 66 (2022) 3981-3984.
2. Cioatera, N., Voinea, E.A., Osiceanu, P., Papa, F., Duta, A., Resceanu, I., Spinu, C.I., Solid State Ionics 339 (2019) 114995.

A COMPREHENSIVE STUDY ON THE PARAMETERS AFFECTING MAGNESIUM PLATING/STRIPPING KINETICS IN RECHARGEABLE Mg BATTERIES

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One of the fundamental concerns for rechargeable Mg batteries (RMB) are electrolyte decomposition and subsequent formation of ionically passivating interphase on Mg anode, that denies further Mg plating and hence affect rechargeability [2, 4]. While Grignard reagents enabled the first prototype of RMB [1], they were impractical for further technology development due to small potential window, corrosiveness and the complexity of processing. Developing Mg electrolytes, that offer (1) wide electrochemical stability window, (2) ease of processing with conventional salts; still able to produce (3) low voltage hysteresis between Mg plating/stripping and (4) high coulombic efficiency for RMBs are in great demand. To ensure these outcomes, a thorough investigation of the interphase between a Mg metal anode and electrolyte is of critical worth as it can dictate stability and reversibility for a particular electrode/electrolyte combination [3]. In this study, we have explored various parameters, such as electrolyte composition and concentration, solvent and substrate nature etc. to understand their effect on Mg plating/stripping kinetics and Coulombic efficiency. We have achieved significant improvement in terms of kinetics by using commercial magnesium bis(trifluoromethanesulfonyl)imide salt ($Mg(TFSI)_2$) and titanium (Ti) substrate with similar crystal structure and lattice parameter as Mg leading to lower nucleation overpotential. Low salt concentration electrolyte and addition of dibutyl magnesium ($Mg(butyl)_2$) also enabled the formation of thinner interphase, richer in solvent based decomposition products, further improving Mg plating kinetics. This work also highlights the complex role of $Mg(butyl)_2$, often considered as a simple drying agent, and how it impacts ion solvation favoring the mobility of electroactive cationic species, paving the way towards better electrolyte design with improved cation transference number.

Key words: Rechargeable magnesium battery, metal anode, plating/stripping, electrolyte

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References

1. Aurbach et al. Nature 2000, 407, 424-427.
2. Li et al. Nat. Rev. Mater., 2020, 5, 276–294.
3. Popovic, Nat Commun 2021, 12, 6240.
4. Wetzel et al. ACS Appl. Mater. Interfaces, 2015, 7, 18406–18414.

MOF-DERIVED TRANSITION METAL OXIDES FOR SMART ENERGY STORAGE DEVICES

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In the 21st century, the rising necessity for energy conservation, alternative energy sources and intelligent electronic devices propels us toward a green sustainable future where electrochromic (EC) devices are poised to be indispensable. Our work explores this intriguing field of electrochromism, where materials change their color in response to electrochemical redox reactions - a notion with promising applications in electrochemical energy storage devices. Consider having a battery/supercapacitor that visibly conveys its charge storage level via color changes, like a real-time indicator. Among potential EC materials, transition metal oxides (TMOs) have received immense attention due to their multiple oxidation states, diversity in morphological characteristics, environmentally benign nature, natural abundance, chemical and environmental stability. However, their electrochemical performances are often retarded by poor charge transfer and ion diffusion kinetics. Nanostructured TMOs help to overcome these issues to some extent as their high surface-to-volume ratio can significantly shorten charge diffusion distances.

Metal-organic framework (MOF) derived carbon embedded porous NiO was synthesized as an EC material, which was integrated as a smart positive electrode in a rechargeable Zn-NiO EC battery, comprising 1 M KOH with 10 mM $ZnAc_2$ as the electrolyte. It delivers an average voltage of ~ 1.85 V and demonstrates a specific capacity of ~ 85.3 mAh/m^2 at 0.1 mA/cm^2 current density. The battery dynamically demonstrates its state of charge by changing the color from dark brown (charged) to transparent (discharged) [1]. However, the color change here is monochromatic and in the context of smart energy storage, it is always desirable to have several shades of color for uniquely identifying the state of charge of the devices. Hence, MOF-derived porous V_2O_5 was subsequently synthesized which could show both cathodic and anodic coloration. The material was eventually integrated into a multi-colored EC asymmetric supercapacitor module with EC polyaniline as the positive electrode, containing 1 M $LiClO_4$/PC as electrolyte. The device demonstrates a high coloration efficiency of 137.2 cm^2/C, an areal capacitance of 12.27 mF/cm^2 and an energy density of 2.21×10^{-3} mWh/cm^2 at a current density of 0.05 mA/cm^2 [2]. By incorporating color-changing capabilities, we hope to improve user experience and bring a sense of fun to energy storage. Such a design of energy storage devices will have promising practical applications in aesthetically pleasing, futuristic, energy-efficient electronic devices in line with modern green technology trends.

Key words: Electrochromism, Transition metal oxide, Battery, Supercapacitor, Smart energy storage

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References

1. Dewan A., Sur S., Narayanan R., Musthafa M., *ChemElectroChem*., 9, e202200001 (2022)
2. Dewan A., Narayanan R., Musthafa M., *Nanoscale*, 14, 17372-17384 (2022)

POLYMER ELECTROLYTES MEMBRANES FOR HIGH-STABLE SOLID-STATE BATTERIES

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The development of clean and efficient energy storage systems is imperative due to the growing energy crisis and its impact on the environment. Li-ion batteries are the most widely used type of energy storage technology because of their high volumetric and gravimetric energy densities. Unfortunately, the current energy densities of intercalation-based Li-ion batteries are insufficient to meet the demands of long-distance mobility. Furthermore, there are safety risks associated with the use of flammable liquid electrolytes in Li-ion batteries, particularly in larger batteries used for grid and electric vehicle (EV) applications. Therefore, solid-state lithium batteries (SSLBs) with solid state electrolytes are highly desirable compared to conventional Li-ion batteries, due to several advantages, such as higher energy density, longer cycle life, and improved safety, among others.

Solid polymer electrolytes (SPEs) are among the most promising solid-state electrolytes; their excellent cycle life, flexibility, and wide operating temperature range have raised significant interest. In the meantime, the SPE can prevent battery short circuits by effectively suppressing the growth of Li dendrites[1-3]. In this study we synthesized and characterized two types of solid molecular polymer electrolytes (SMICE and SICPE) chemically, physically, thermodynamically, and electrochemically. This was done to establish the relationship between the chemical structure of the system, its composition, and its electrochemical properties in order to develop an improved solid-state battery with enhanced characteristics.

Following electrochemical tests, the symmetric cells exhibited long-term cycling stability at 25°C for 350 and 650 hrs. before electrochemical degradation occurred. When the cell was cycled at 60°C using a current density of 0.1 mA/cm^{-2}, it withstood over 1000 hrs. These measurements demonstrate excellent compatibility of the developed polymeric membrane with Li metal even at higher temperatures.

Key words: Polymer electrolytes, Solid state, Lithium-ion batteries, Ionic conductivity

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Romanian Ministry of Research, Innovation, and Digitalization under projects PN 23 15 02 01, BatNaS and PN 23 15 02 02, PrisPEC.

References

1. Kim, J.-K., Lim, Y.J., Kim, H., Cho, G.-B., Kim, Y., A hybrid solid electrolyte for flexible solid-state sodium batteries, *Energy Environ. Sci*., 8 (2015) 3589–3596.
2. Zhang, W., Nie, J., Li, F., Wang, Z.L., Sun, C., A durable and safe solid-state lithium battery with a hybrid electrolyte membrane, *Nano Energy*, 45 (2018) 413–419.
3. Wang, Y., Richards, W.D., Ong, S.P., Miara, L.J., Kim, J.C., Mo, Y., Ceder, G., Design principles for solid-state lithium superionic conductors, *Nat. Mater.,* 14 (2015) 1026–1031.

TRIS(TRIMETHYLSILYL) BORATE AS ELECTROLYTE ADDITIVE TO MITIGATE THE FAILURE MODES OF $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) - BASED LITHIUM-ION POUCH CELLS

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Lithium-ion batteries with high energy density cathodes based on nickel-rich layered oxide materials have gained significant attention due to their higher reversible capacity with increasing Ni content at the same cut-off voltage. Nickel-rich materials have become the state-of-the-art cathode materials in commercial LIBs for automotive applications, demonstrating substantially improved energy density [2] In particular, $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) provides a good compromise often electrochemical performance, high energy densities and cost. However, these Ni-rich cathodes always suffer from rapid capacity degradation induced by an unstable cathode-electrolyte interphase (CEI) layer, which is composed of inorganic salts, transition metals, lithium ions, a small number of organic compounds, and other components [1, 3]. Therefore, the presence of an effective CEI with high ionic conductivity low electronic conductivity, stable mechanical structure, and chemical stability is significant for inhibiting detachment or cracking during the volume changes of cathode materials, and it cannot be disregarded [4]. Consequently, the simplest and most economical strategy for improving the cycling stability of the NMC 811 cathode is the use of new electrolyte formulations that include additives. In this study, boron compound as tris(trimethylsilyl) borate (TMSB) was used as additive in the benchmark electrolyte consisting of 1M $LiPF_6$ in EC/DMC (1:1) with the aim of understanding the structure-performance relationship of NMC811 cathodes and the newly developed electrolytes. The influence of the electrolyte additives on cycling stability and Coulombic efficiency was evaluated in NMC811/Graphite pouch cells configuration.

Key words: Lithium-ion battery, electrolyte additive, nickel-manganese-cobalt (NMC811), tris(trimethylsilyl) borate

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References

1. Ekaterina Laakso, Sofya Efimova, Mattia Colalongo, Pertti Kauranen, Katja Lahtinen, Emilio Napolitano, Vanesa Ruiz, Joze Moskon, Miran Gaberscek, Juyeon Park, Steffen Seitz, Tanja Kallio, *Journal of Power Sources* 599 (2024) 234159;
2. Wangda Li, Evan M. Erickson, Arumugam Manthiram, *Nature Energy* 5 (2020) 26–34;
3. Tianyu Li, Xiao-Zi Yuan, Lei Zhang, Datong Song, Kaiyuan Shi, Christina Bock, *Electrochemical Energy Reviews* 3 (2020) 43–80;
4. Nan Zhang, Bo Wang, Fan Jin, Yong Chen, Yunpeng Jiang, Changyuan Bao, Jiyu Tian, Jingyang Wang, Ruoyu Xu, Yaohua Li, Qiang Lv, Huaizheng Ren, Dianlong Wang, Huakun Liu, Shixue Dou, Xiang Hong, Cell Reports Physical Science 3 (2022) 101197.

TOWARD ENHANCED LONG CYCLING STABILITY IN *LNMO* Li-ION POUCH CELLS VIA CARBONATE-BASED ELECTROLYTES WITH ADDITIVES

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High-voltage spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) is a promising cathode material for the next generation of high-performance lithium-ion batteries (LIBs) due to its high energy density [1], high operating voltage (~4.7 V vs. Li^+/Li), cobalt-free composition, environmentally friendly characteristics, and cost-effective production. The exclusion of cobalt (Co) from the cathode material offers significant benefits, including reduced costs, lower toxicity risks, and improved sustainability. LNMO has attracted considerable attention in the advancement of lithium-ion battery technology due to its favorable electrochemical properties [2]. This study explores the use of LNMO as a cathode material and graphite as an anode material in a pouch cell configuration. The research analyzes the electrochemical performance and structural stability of LNMO under various operating conditions. Electrochemical characterization methods, including galvanostatic testing at different temperatures and electrochemical impedance spectroscopy (EIS), are used to reveal the electrochemical behavior of LNMO in pouch cells configuration. The research focuses on the analysis and manufacturing of LNMO cathodes and graphite anodes in Li-ion pouch cell configuration. The study assesses the electrochemical performance of these cells by characterizing them with carbonate-based electrolytes containing additional additives within a voltage range of 3.0 to 4.9V. Through extensive long-term cycling tests, the Li-ion pouch cells demonstrated enhanced electrochemical stability at high voltages, maintaining a capacity retention of over 80% after 2300 cycles at a 1C rate, with no gas evolution associated with electrolyte degradation at high voltage. Additionally, these cells achieved an average coulombic efficiency of 99%.

Key words: Lithium-ion batteries, $LiNi_{0.5}Mn_{1.5}O_4$, High voltage spinel, High energy density, Electrochemistry

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References

1. Daniele V., Roberto C., Giorgio Montinaro, Mihaela Buga, Noelia Cortes Felix, Gary Evans, Federico Bella, Julia Amici, Carlotta Francia, Silvia Bodoardo, Tailoring cathode materials: A comprehensive study on LNMO/LFP blending for next generation lithium-ion batteries, Journal of Power Sources 613 (2024) 234955.
2. Chengjie Yina, Zhiqiang Bao, Hui Tan, Hongming Zhoua, Jian Li, Metal-organic framework-mediated synthesis of LiNi0.5Mn1.5O4: Tuning the Mn3+ content and electrochemical performance by organic ligands, Chemical Engineering Journal 372 (2019) 408–419.

SIMPLE DRY-PROCESS FOR SOLVENT-FREE $Na_3V_2(PO_4)_3$ CATHODE: APPROACH FOR ENHANCED SUSTAINABILITY

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Conventional methods for synthesizing sodium-ion battery electrodes frequently involves solvent-based procedures, which raise environmental concerns due to solvent toxicity and disposal issues, as well as increasing production costs.

By eliminating the hazardous organic solvents that are typically required for the slurry preparation of electrode materials, the cathode synthesis process reduces environmental impact while also simplifying the manufacturing process.

In this research work, we focused on the development and characterization of a solvent-free $Na_3V_2(PO_4)_3$ cathode, optimized for high energy density and long cycle life. This method of producing electrodes entails combining powdered electrochemically active materials with a small amount of dry polytetrafluoroethylene (PTFE) binder, without the need for a solvent, to prepare an electrode[1].

We successfully developed a sodium cathode with good cycle performance, large specific capacity, and excellent electrochemical stability through precise control of material composition and thermal processing.

The galvanostatic cycling of half-cells using the synthesized electrode as the cathode and Na metal as the reference electrode[2] was conducted at different C-rates. The preliminary results indicate that the solvent-free sodium cathode delivers a specific capacity of around 98mAh/g, along with high coulombic efficiency and minimal capacity fade after 100 cycles. This process not only improves the environmental profile of sodium-ion batteries but also has the potential to reduce production costs on a large scale.

Key words: Sodium Battery, Solvent-free, Cathode, Stability, Synthesis

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References

1. Westman, Kasper, et al. "Diglyme based electrolytes for sodium-ion batteries." ACS Applied Energy Materials 1.6 (2018): 2671-2680.
2. Li, Yongxing, et al. "Progress in solvent-free dry-film technology for batteries and supercapacitors." Materials Today 55 (2022): 92-109.

HIGH-VOLTAGE DEGRADATION OF *NASICON*-TYPE $Na_3V_2(PO_4)_3$ POLYANIONIC CATHODE MATERIAL

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Direct measurement of the voltage of both working and counter electrodes cannot be made for a two-electrode system. Instead, voltages are inferred from the full-cell voltage and previous knowledge of the precise chemical system, including 3-electrode tests. When used in real-world applications, individual cells (or particles within the cathode) can routinely and randomly be pushed outside their design voltages without any way of immediately knowing. This is often a result of ageing or abuse during operation [1]. These extreme potentials can be responsible for the dissolution of transition metals, which can travel from the cathode and integrate into the forming SEI at the anode, greatly enhancing the depletion of active shuttling ions [2].

In this poster, I will present direct evidence for the chemo-mechanical break-up of a standard $Na_3V_2(PO_4)_3$ (NVP) cathode particle when cycled to varying extended Upper cut-off voltages (UCVs), ranging from 3.8V to 4.8V. X-ray images of the particles were obtained *in operando* throughout charging at Diamond Light Source's I-14 X-ray nanoprobe beamline. 2D maps of the Vanadium distribution show the particles' expansion and enhanced physical degradation when pushed above its standard UCV of 3.8V. XANES maps, spatially resolved down to 50nm, were taken of the V K-edge to correlate any changes in morphology with precise Vanadium chemistry but showed no phase separation or meaningful heterogeneities.

To understand the effects of extended UCVs on NVP more completely, further *ex-situ* investigations are being carried out, including an advanced 3D-Ptychography-XANES-nanoCT study at Diamond's I13-1 beamline, which will be presented as future work.

Key words: Sodium-ion Battery; High voltage; Degradation; Synchrotron: Nano-probe

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References

1. Wang, Z., Hong, J., Liu, P. & Zhang, L. (2017) *Applied energy*. 196, 289–302.
2. Gilbert, J.A., Shkrob, I.A. & Abraham, D.P. (2017) *Journal of the Electrochemical Society*. 164 (2), A389.

REVISITING TIN OXIDE ANODES WITH A SCALABLE NANOSCALE FABRICATION PROCESS

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For nearly 30 years, the reliable use of conversion and alloying materials as high-capacity electrodes in Li-ion batteries has largely remained an elusive goal. One notable success was Sony's commercialization of the Tin-based Nexelion™ chemistry in 2005. Despite the limited range of commercialized systems, the scientific literature on this topic remains vibrant, driven by the promise of specific capacities exceeding 1000 mAh/g. However, conversion/alloy systems face well-known challenges: extremely poor first cycle efficiencies, large voltage hysteresis, and poor cyclability due to significant morphological changes during cycling. Nano structuring is widely considered the best approach to mitigating these issues. Within the SMICE-Li Project, we have revisited conversion-alloy materials using a scalable synthesis route. A systematic study on doped and undoped SnO_2, examining the effects of different dopants, particle sizes, and cycling voltage windows was carried out. Our findings reveal clear differences in cyclability based on particle size and significant performance variations between different dopants (Ni, Fe, Co, Mn).

Key words: Conversion-Alloy anodes, Tin oxide, Lithium-ion batteries

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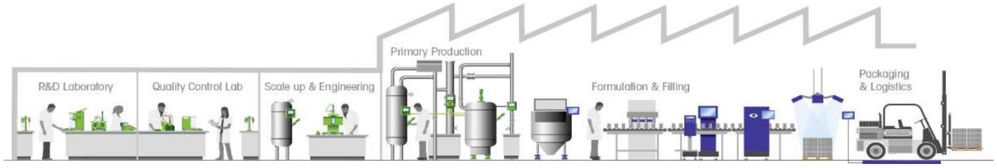

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