FRIEDRICH-SCHILLER-
UNIVERSITÄT
JENA

Faculty of Chemistry and
Earth Sciences

ORGANIC BATTERY DAYS 2019

Scientific Programme

3 - 5 June 2019 | Jena (Germany)

POWER IN ANY SHAPE YOU CAN IMAGINE: TAeTTOOz®

Create batteries like
TAeTTOOz®

TAeTTOOz® materials for printable, fully polymer-based batteries deliver a host of benefits for both you and your products:

1. Design freedom
2. Flexible use
3. Seamless integration
4. Free of toxic substances
5. Rechargeability
6. Scalable production

EVONIK CREAVIS GMBH
Paul-Baumann-Strasse 1
45772 Marl
Germany

www.evonik.com
www.taettooz.com

EVONIK
POWER TO CREATE

TABLE OF CONTENTS

GENERAL INFORMATION

Date
3 - 5 June 2019

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

Unless otherwise indicated, the events will take place in the lecture hall of the Center for Applied Research (ZAF), Philosophenweg 7, 07743 Jena, Germany.

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

Scientific Advisory Board
Prof. Dr. Matthieu Becuwe
(Amiens/FR)
Prof. Dr. Daniel Brandell
(Uppsala/SE)
Prof. Dr. Jun Chen
(Tianjin/CN)
Prof. Dr. Ji Eon Kwon
(Seoul/KR)
Prof. Dr. Kenichi Oyaizu
(Tokyo/JP)
Prof. Dr. Ho Seok Park
(Suwon-si/KR)
Prof. Dr. Philippe Poizot
(Nantes/FR)
Prof. Dr. Ulrich S. Schubert, Chairman
(Jena/DE)
Dr. Masaru Yao
(Tokyo/JP)
Prof. Dr. Yan Yao
(Houston/US)

WELCOME NOTE

Dear friends and colleagues,

it is my great pleasure to welcome you to the Organic Battery Days 2019, the only international conference in the emerging field of Organic Batteries this year.

I am looking forward to three days of excellent scientific exchange and networking with international experts from science, research, politics, administration and industry to exchange knowledge and experience on the latest developments in the field of electro-chemical energy storage based on organic active materials, including:

- Organic cathode materials for high performance organic metal-ion batteries.
- Organic anode materials.
- Active materials for metal-sulfur batteries.
- Biomass-derived organic electrode materials for sustainable batteries.
- Novel liquid and polymer electrolytes for organic batteries.
- Novel active materials and concepts for metal-free redox flow batteries.
- Characterization of active materials and interfaces.
- Computational chemistry for material design and understanding.
- Novel device architectures for organic batteries (fully printable, stretchable, single-use, ultra-low temperature, ...).

After two days of oral and poster presentations that will be opened by one of the inventors of organic batteries, Prof. Dr. Hiroyuki Nishide, the conference programme will be rounded off on Wednesday by hands-on workshops as well as a preparation meeting for our new DFG Priority Programme SPP 2248 on polymer-based batteries.

Sincerely yours

Ulrich Schubert

Prof. Dr. Ulrich S. Schubert

SPONSORS AND EXHIBITORS

Gold Sponsors

Bio-Logic Science Instruments

Evonik Creavis GmbH

Sciospec Scientific Instruments GmbH

Silver Sponsors

C3 Prozess- und Analysentechnik GmbH

Neware Technology Limited

Bronze Sponsors

NETZSCH-Gerätebau GmbH

Chemspeed Technologies AG

Other Sponsors

Wirtschaftsförderungs-gesellschaft Jena mbH

SPONSORS AND EXHIBITORS

Funding Agencies

Deutsche Forschungsgemeinschaft
German Research Foundation

Deutsche Forschungs-gemeinschaft e.V.

Ernst Abbe Stiftung

Ernst-Abbe-Stiftung

Supporting Societies

EuChemS
European Chemical Society

European Chemical Society (EuChemS)

International Society of Electrochemistry
ISE

International Society of Electrochemistry (ISE)

Media Partners

ACS Energy Letters

ACS Publications

ADVANCED ENERGY MATERIALS

WILEY-VCH Verlag G mbH & Co. KGaA

SCIENTIFIC PROGRAMME

Monday, 3 June 2019

08:30 am	REGISTRATION
09:30 am	CONFERENCE OPENING
	Welcome notes *Prof. Dr. Ulrich S. Schubert* *Chairman* *Friedrich Schiller University Jena, Jena (DE)*
	Wolfgang Tiefensee *Thuringian Minister of Economic Affairs, Science and Digital Society, Erfurt (DE)*
	Prof. Dr. Alexander Brenning *Dean of the Faculty of Chemistry and Earth Sciences,* *Friedrich Schiller University Jena, Jena (DE)*
10:00 am	PLENARY LECTURE Radical polymers as an organic charge-transport and energy-storage material *Prof. Dr. Hiroyuki Nishide* *Waseda University, Tokyo (JP)*
10:50 am	INVITED LECTURE Innovative sulfur containing polymers for batteries *Prof. Dr. David Mecerreyes* *Polymat, University of the Basque Country UPV/EHU, San Sebastián (ES)*
11:25 am	INVITED LECTURE Cycle-stable, high capacity metal-sulfur batteries based on sulfur/poly(acrylonitrile) (SPAN) cathodes *Prof. Dr. Michael Buchmeiser* *University of Stuttgart, Stuttgart (DE)*

SCIENTIFIC PROGRAMME

12:00 pm — CONTRIBUTED LECTURE

Exploring organically modified sulfur copolymer / CNT network cathode for Li-S batteries

Dr. Soumyadip Choudhury

Technische Universität Chemnitz, Chemnitz / Leibniz Institute of Polymer Research Dresden , Dresden (DE)

12:20 pm — LUNCH BREAK

01:20 pm — PROJECT PRESENTATION

DFG Priority Programme SPP 2248 - Polymer-based batteries

Prof. Dr. Ulrich S. Schubert

Friedrich Schiller University Jena, Jena (DE)

01:45 pm — INVITED LECTURE

Tailoring dihydroxyterephthalate unit toward organic lithiated positive electrode materials with high redox potentials

Dr. Franck Dolhem

University of Picardie Jules Verne, Amiens (FR)

02:20 pm — CONTRIBUTED LECTURE

S-Tetrazine as a new redox center for high-performance electrode materials in rechargeable batteries

Prof. Dr. Ji Eon Kwon

Seoul National University, Seoul (KR)

02:40 pm — CONTRIBUTED LECTURE

Natural quinones as sustainable battery cathodes

Dr. Clemens Liedel

Max Planck Institute of Colloids and Interfaces, Potsdam (DE)

SCIENTIFIC PROGRAMME

03:00 pm — CONTRIBUTED LECTURE

Poly(catechol) nanoparticles and their redox activity
Dr. Klemen Pirnat
National Institute of Chemistry, Ljubljana (SI) / Polymat, University of the Basque Country UPV/EHU, San Sebastián (ES)

03:20 pm — SPONSORED LECTURE

The development of a fully printable energy storage technology
Dr. Andreas Wild
Evonik Creavis GmbH, Marl (DE)

03:55 pm — COFFEE BREAK

04:25 pm — CONTRIBUTED LECTURE

Crystallographic change behavior of 2,5-dimethoxy-1,4-benzoquinone during charge and discharge
Dr. Hikaru Sano
National Institute of Advanced Industrial Science and Technology (AIST), Osaka (JP)

04:45 pm — CONTRIBUTED LECTURE

Cathode performances of porous organic crystals formed by charge-transfer interactions
Prof. Dr. Hirofumi Yoshikawa
Kwansei Gakuin University, Nishinomiya (JP)

05:05 pm — CONTRIBUTED LECTURE

Empowering organic-based negative electrode material through molecular design
Dr. Matthieu Becuwe
University of Picardie Jules Verne / Institut de Chimie de Picardie (ICP), Amiens (FR)

SCIENTIFIC PROGRAMME

05:25 pm

INVITED LECTURE

Molecular electrode materials from nature – design of a green battery
Prof. Dr. George John
The City College of New York, New York (US)

06:00 pm

SHORT POSTER PRESENTATIONS

Isoindoline nitroxide derived high-voltage cathode materials
Dr. James P. Blinco
Queensland University of Technology, Brisbane (AU)

Development of high solubility catholytes for organic aqueous redox flow batteries
Dr. Emil Dražević
Aarhus University, Aarhus (DK)

A novel binder-free cathode based on electro-polymerized conductive polymer for Li-S batteries
Dr. Shilin Mei
Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin (DE)

Structure-property relations of quinone-based active materials for redox flow batteries
Prof. Dr. Doreen Mollenhauer
Justus-Liebig University Giessen, Giessen (DE)

Printable gel polymer electrolyte for all-organic batteries
Simon Münch
Friedrich Schiller University Jena, Jena (DE)

Reduced graphene oxide /poly (pyrrole-*co*-thiophene) composite framework for energy storage in supercapacitors
Prof. Dr. Anwar-ul-Haq Ali Shah
University of Peshawar, Peshawar (PK)

SCIENTIFIC PROGRAMME

06:20 pm to 07:50 pm	POSTER SESSION AND DRINKS *Lecture hall and foyer*
07:15 pm	SCIENTIFIC ADVISORY BOARD MEETING *Conference Room CEEC Jena (E 009), Philosophenweg 7a, 07743 Jena*

SCIENTIFIC PROGRAMME

Tuesday, 4 June 2019

09:00 am — INVITED LECTURE
Understanding superlithiation of organic electrode materials by evolutionary algorithm DFT calculations
Prof. Dr. Daniel Brandell
Uppsala University, Uppsala (SE)

09:35 am — INVITED LECTURE
Progress in all-organic rechargeable batteries using the anionic cell configuration
Prof. Dr. Philippe Poizot
University of Nantes, Nantes (FR)

10:10 am — CONTRIBUTED LECTURE
Radical polymer/carbon nanotube hybrids for ultra-thin, stretchable, and solid-state batteries
Dr. Kan Hatakeyama-Sato
Waseda University, Tokyo (JP)

10:30 am — CONTRIBUTED LECTURE
Aqueous batteries based on polyimide and prussian blue analogues
Prof. Dr. Anders Bentien
Aarhus University, Aarhus (DK)

10:50 am — COFFEE BREAK

11:20 am — INVITED LECTURE
(Hetero)aromatic redox polymers as electrode-active materials for organic batteries
Prof. Dr. Birgit Esser
University of Freiburg, Freiburg (DE)

11:55 am — CONTRIBUTED LECTURE
Full organic-based aqueous battery with millimeter-thick electrodes
Dr. Joel Gaubicher
University of Nantes, Nantes (FR)

SCIENTIFIC PROGRAMME

12:15 pm	CONTRIBUTED LECTURE Development of organic electrode materials for anion-ion batteries *Dr. Lionel Dubois* *Université Grenoble Alpes, Grenoble (FR)*
12:35 pm	CONTRIBUTED LECTURE Biodegradable single-use organic batteries for small-sized electronic devices *Dr. Juan Pablo Esquivel* *Institute of Microelectronics of Barcelona (IMB-CNM), Barcelona (ES)*
12:55 pm	LUNCH BREAK
02:00 pm	CONTRIBUTED LECTURE Ultra-low temperature battery based on non-metal design *Prof. Dr. Hui Zhan* *Wuhan University, Wuhan (CN)*
02:20 pm	INVITED LECTURE Consideration on the preparation and application of carbonyl electrode materials *Prof. Dr. Jun Chen* *Nankai University, Tianjin (CN)*
02:55 pm	INVITED LECTURE Gel electrolytes for organic batteries *Dr. Alexandra Lex-Balducci* *Friedrich Schiller University Jena, Jena (DE)*
03:30 pm	CONTRIBUTED LECTURE The influence of the electrolyte composition on the electrochemical performance of organic batteries *Prof. Dr. Andrea Balducci* *Friedrich Schiller University Jena, Jena (DE)*

Bio-Logic EIS Quality Indicators

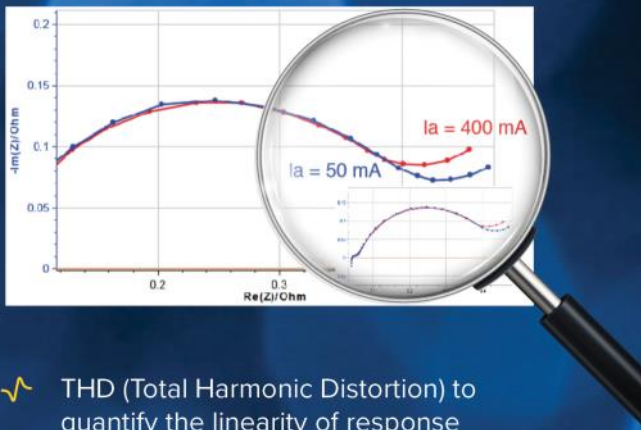
Pain-free EIS

EIS is a powerful scientific tool that identifies vital data relating to redox processes: information that can open up exciting scientific and industrial opportunities.

However, this data can be as difficult to manage as it is valuable, and the **delicate balancing act of managing linearity and time-variance** can pose problems for even the most experienced of experts.

Bio-Logic's quality indicators simplify and validate impedance experiments and drive you straight to the data you need.

Two curves.
But which one is correct?



- THD (Total Harmonic Distortion) to quantify the linearity of response
- NSD (Non-Stationary Distortion) indicates the effect of time variance and transient regime
- NSR (Noise to signal ratio) ensures that the signal is large enough in relation to measurement noise

EIS doesn't need to be painful

Video tutorial at www.bio-logic.net

BioLogic
Science Instruments

SCIENTIFIC PROGRAMME

03:50 pm	INVITED LECTURE Design for long cycle-life quinone-type active materials by oligomerization *Dr. Masaru Yao* *National Institute of Advanced Industrial Science and Technology (AIST), Osaka (JP)*
04:25 pm	COFFEE BREAK
04:55 pm	INVITED LECTURE Metal-free and membrane-free redox flow batteries by using immiscible electrolytes based on organic redox molecules *Dr. Rebeca Marcilla* *IMDEA Energy Institute, Madrid (ES)*
05:30 pm	CONTRIBUTED LECTURE Further investigations of the electrode/electrolyte interface of organic electrode materials for Li-ion batteries *Dr. Stéven Renault* *University of Nantes, Nantes (FR)*
05:50 pm	CONTRIBUTED LECTURE Insight into solid-state electrochemistry of bi-redox organic battery materials *Alae Eddine Lakraychi* *Catholic University of Louvain, Louvain-la-Neuve (BE)*
06:10 pm	INVITED LECTURE Redox-active polymer based nano-objects via polymerization induced self-assembly *Prof. Dr. Jean-François Gohy* *Catholic University of Louvain, Louvain-la-Neuve (BE)*

SCIENTIFIC PROGRAMME

06:45 pm

FAREWELL AND AWARD OF THE WINNERS OF THE POSTER PRIZES

Prof. Dr. Ulrich S. Schubert
Friedrich Schiller University Jena, Jena (DE)

Prof. Dr. Andrea Balducci
Friedrich Schiller University Jena, Jena (DE)
International Society of Electrochemistry (ISE)

SCIENTIFIC PROGRAMME

Wednesday, 5 June, 2019 (parallel sessions)

10:00 am	WORKSHOPS Introduction in organic batteries: basic principles of organic batteries *Conference Room CEEC Jena (E 009), Philosophenweg 7a, 07743 Jena* Hands-on workshop I Electrode preparation and pouch cell assembly Hands-on workshop II Characterization techniques for organic batteries
10:00 am	PROJECT PLANNING Preparation meeting for the DFG Priority Programme SPP 2248 - Polymer-based batteries *Short presentations of interested scientists and groups from Germany*
01:30 pm	LUNCH BREAK
02:30 pm	END OF CONFERENCE

SOCIAL PROGRAMME

Monday, 3 June 2019

08:00 pm

CONFERENCE DINNER

Botanical Garden Jena
Enjoy a memorable evening in the relaxed atmosphere of the "green lung of Jena"!

Tuesday, 4 June 2019

07:00 pm

THURINGIAN BARBECUE

Center for Energy and Environmental Chemistry Jena (CEEC Jena)
Thuringia is world famous for its "Bratwurst"! Enjoy a typical Thuringian barbecue evening with us - including stimulating conversations with colleagues and friends.

Abstracts of Oral Contributions

ABSTRACTS OF ORAL CONTRIBUTIONS

Radical polymers as an organic charge-transport and energy-storage material

H. Nishide
Research Institute for Science and Engineering, Waseda University, Tokyo 169-8555, Japan
nishide@waseda.jp

A breakthrough made for the charge-transporting and -storing organic materials by the use of radical polymers is described. The organic radical polymers are a series of polymers bearing robust nitroxides, triaryl aminiums, phenoxyls, etc as electron-releasing and -gaining sites per their repeating unit. They are characterized by both a dense population of the radical redox site and an amorphous plasticized state with the coexistence of small amount of electrolytes, to allow very fast self-exchanging reaction among the sites with the driving force of steep concentration gradient, and to provide efficient charge-transport and -storage throughout the polymers. The very high charge-transporting capability, i.e. redox conduction, within the purely organic polymers led to the tremendously large current density beyond 100 mA/cm² and the electrical conducting for the long distance of 50 μm. Chemical bistability of the reduced and oxidized species of radical polymers permits both ultimate energy density and durable cyclability in charging and discharging. Various types of batteries were fabricated with the radical polymers as the electrode-active materials. Output voltage of the batteries is fluctuating-free, corresponds to their redox potential difference, and is tunable with their molecular designing. The batteries provide burst power, which also allows instant full charging in a few seconds. The ultrafast electrode-activity of radical polymers was also tested as an adhesive additive in the conventional Li ion batteries. The radical polymers were also examined as the charge-transporting mediator in photovoltaic and water-splitting cells and as the hydrogenation/dehydrogenation site for a hydrogen-carrier. Organic radical polymer-based devices are, of course, characterized by the inherent advantages of flexible, even stretchable, resource-unlimited, and environmentally benign properties.

ABSTRACTS OF ORAL CONTRIBUTIONS

Innovative sulfur containing polymers for batteries

D. Mecerreyes, N. Casado, I. Gomez
POLYMAT University of the Basque Country UPV/EHU, Centro Joxe Mari Korta, Avenida Tolosa 72 Donostia-San Sebastian 20018, Spain
david.mecerreyes@ehu.es

Polymers play an important role in the development of future battery technologies. Nowadays, new ion conducting polymers or polymer electrolytes, electrically conductive polymers and redox polymers are highly investigated in several battery technologies such as metal-air, redox-flow, printable batteries, sodium, magnesium or different battery chemistries.[1] Polymers can be used in different parts of the battery such as redox active cathodic material, polymer electrolyte or polymeric binders.
In this lecture we will discuss our recent activities in the development of innovative polymers for Electrochemical Energy Storage. In particular, we will present the main synthetic and characterization methods as well as applications of Redox Polymers. Our recent activities related to the development of new redox active sulfur copolymers for lithium-sulfur batteries will be discussed. The talk will include the inverse vulcanization of sulfur using natural dienes, the synthesis of sulfur rich poly(anthraquinonyl sulfides) and the combination of sulfur polymers and poly(ionic liquid)s.

References
[1] N. Casado, G. Hernandez, H. Sardon, D. Mecerreyes, *Prog. Polym. Sci.* **2016**, *52*, 107-135.
[2] a) I. Gomez, O. Leonet, J. A. Blazquez, D. Mecerreyes, *ChemSusChem* **2016**, *9*, 3419-3425.
b) I. Gomez, D. Mantione, O. Leonet, J. A. Blazquez, D. Mecerreyes, *ChemElectroChem* **2018**, *2*, 260-265.
c) I. Gomez, O. Leonet, J. A. Blazquez, H. J. Grande, D. Mecerreyes, *ACS Macro Lett.* **2018**, *7*, 419-424.
d) I. Gomez, A. Fernandez de Anastro, O. Leonet, J. A. Blazquez , H. J. Grande, J. Pyun, D. Mecerreyes, *Macromol. Rapid Commun.* **2018**, submitted.

ABSTRACTS OF ORAL CONTRIBUTIONS

Cycle-stable, high capacity metal-sulfur batteries based on sulfur/poly (acrylonitrile) (SPAN) cathodes

M. R. Buchmeiser
Chair of Macromolecular Compounds and Fiber Chemistry, Institute of Polymer Chemistry, University of Stuttgart, Germany
michael.buchmeiser@ipoc.uni-stuttgart.de

Lithium-sulfur (Li-S) and magnesium-sulfur (Mg-S) batteries are among the most promising next-generation energy storage systems.[1] Despite a lower operating voltage in Mg-S batteries compared to Li-S batteries, Mg-S batteries offer a higher volumetric energy density and higher safety. Generally, conventional metal sulfur batteries require high amounts of redox-inactive liquid electrolytes, which do not contribute to cell capacity. Thus, the practical specific energy of these batteries is often comparably poor (≤500 Wh/kg) and barely competitive with existing, high-end Li-ion batteries. This talk will address the latest accomplishments in both, Li- and Mg-S batteries. Generally, sulfurized poly (acrylonitrile) (SPAN) was used as cathode materials. In contrast to most other cathode materials, it contains sulfur chemically bound to a semiconductive polymeric matrix. The special nature of SPAN with its vinylogous/phenylogous enolic thioamides allows for a cycle-stable discharge/charge over more than 1200 cycles up to rates of 8C. Hybrid metal-sulfur batteries that contain both a liquid and a solid cathode, i.e., dimethyl trisulfide (DMTS) and SPAN, have been prepared.[2-6] These exhibit high capacity (formally, when referring solely to the sulfur in the cathode, up to 7100 mA.h/$g_{\text{sulfur of cathode}}$), high areal capacity up to 4.3 mA.h.cm^{-2}, high rate capability up to 8 C and excellent cycle stability (>700 cycles).[7] In addition, both the working and aging mechanism have been elucidated by NMR, Raman, X-ray photoelectron and electronic impedance spectroscopy, X-ray powder diffraction, cyclic voltammetry, and *post-mortem* analysis. Generally, the working and aging mechanisms differ substantially from those of sulfur@carbon cathodes[8] and allow even the use of carbonate-based electrolytes.[9] Implications on Mg-S batteries will be presented, too.

References

[1] X. Ji, K. T. Lee, L. F. Nazar, *Nat. Mater*. **2009**, *8*, 500.
[2] J. Wang, J. Yang, J. Xie, X. Naixin, *Adv. Mater*. **2002**, *14*, 963.
[3] J. Fanous, M. Wegner, J. Grimminger, Ä. Andresen, M. R. Buchmeiser, *Chem. Mater.* **2011**, *23*, 5024.
[4] J. Fanous, M. Wegner, J. Grimminger, M. Rolff, M. B. M. Spera, M. Tenzer, M. R. Buchmeiser, *J. Mater. Chem*. **2012**, *22,* 23240.
[5] J. Fanous, M. Wegner, M. B. M. Spera, M. R. Buchmeiser, *J. Electrochem. Soc.* **2013**, *160*, A1169.
[6] M. Frey, R. K. Zenn, S. Warneke, K. Müller, A. Hintennach, R. E. Dinnebier, M. R. Buchmeiser, *ACS Energy Lett*. **2017**, *2*, 595.

ABSTRACTS OF ORAL CONTRIBUTIONS

[7] S. Warneke, R. Zenn, T. Lebherz, K. Müller, A. Hintennach, U. Starke, R. E. Dinnebier, M. R. Buchmeiser, *Adv. Sust. Syst.* **2018**, *2*, 1700144.
[8] S. Warneke, M. Eusterholz, R. Zenn, A. Hintennach, R. E. Dinnebier, M. R. Buchmeiser, *J. Electrochem. Soc*. **2018**, *165*, A6017.
[9] S. Warneke, A. Hintennach, M. R. Buchmeiser, *J. Electrochem. Soc.* **2018,** *165*, A2093.

ABSTRACTS OF ORAL CONTRIBUTIONS

Exploring organically modified sulfur copolymer / CNT network cathode for Li-S batteries

S. Choudhury[1,2], M. Sommer[1,2]
[1]Professur für Polymerchemie, Technische Universität Chemnitz, Straße der Nationen 62, 09111 Chemnitz, Germany
[2]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Straße 6, 01069 Dresden, Germany
soumyadip.choudhury@chemie.tu-chemnitz.de

Development of economic, scalable and efficient energy storage systems is needed to counterbalance fluctuations of renewable energy generations. Design of novel nanostructures for battery electrodes is key to maximize energy density of batteries and render them economically attractive. Lithium-sulfur (Li-S) batteries are promising as they can reach energy densities comparable to petroleum-based fuels.[1, 2] Li–S batteries encompass a highly promising future generation energy storage system for automotive applications because of high theoretical capacity (1672 mAh/g), and energy (2600 Wh/kg) normalized to sulfur mass. However, the efficient utilization of active sulfur is a prime issue to generate nanostructured, conductive electrodes. Despite of these aspects, repeated cycling in Li–S batteries ultimately leads to very low capacity retention due to leaching of soluble sulfur species into the electrolyte. To alleviate such leaching behavior and to enhance sulfur utilization, inverse vulcanization was proposed to modify the active material i.e. sulfur by diene monomers.[3] In this contribution, S-diisopropylbenzene copolymers are synthesized and combined with high surface area conductive carbon. The mixing process of sulfur-containing copolymers with carbon materials is assisted by shear in a two-roll mill to capitalize on the softened state of the copolymer. This high-throughput mixing method demands carbon with exohedral porous structure with almost no destruction by shear mixing. The organically modified sulfur-based active material and their hybrids with carbon nanotubes and carbon nanotube mats were thoroughly characterized in terms of structure and chemical composition, and finally tested by electrochemical benchmarking. These hybrids yield electrodes with high sulfur content and demonstrate stable electrochemical performances superior to melt-infiltrated reference samples.

References

[1] P. G. Bruce, S. A. Freunberger, L. J. Hardwick, J.-M. Tarascon, *Nat. Mater.* **2011**, *11*, 19-29.
[2] S. Choudhury, P. Srimuk, K. Raju, A. Tolosa, S. Fleischmann, M. Zeiger, K. I. Ozoemena, L. Borchardt, V. Presser, *Sustainable Energy Fuels* **2018**, *2*, 133-146.
[3] A. G. Simmonds, J. J. Griebel, J. Park, K. R. Kim, W. J. Chung, V. P. Oleshko, J. Kim, E. T. Kim, R. S. Glass, C. L. Soles, Y.-E. Sung, K. Char, J. Pyun, *ACS Macro Lett.* **2014**, *3*, 229-232.

ABSTRACTS OF ORAL CONTRIBUTIONS

Tailoring dihydroxyterephthalate unit toward organic lithiated positive electrode materials with high redox potentials

F. Dolhem[1], A. Jouhara[2], A. Lackraychi[1,3,4], N. Dupré[2], D. Guyomard[2], M. Bécuwe[3,4], P. Poizot[2]
[1]Laboratoire de Glycochimie, des Antimicrobiens et des Agroressources (LG2A), UMR CNRS 7378, Université de Picardie Jules Verne, 33 rue Saint-Leu, 80039 Amiens Cedex, France
[2]Institut des Matériaux Jean Rouxel (IMN), UMR CNRS 6502, Université de Nantes, 2 rue de la Houssinière, B.P. 32229, 44322 Nantes Cedex 3, France
[3]Laboratoire de Réactivité et Chimie des Solides (LRCS), UMR CNRS 7374, Université de Picardie Jules Verne, 33 rue Saint-Leu, 80039 Amiens Cedex 1, France
[4]Réseau sur le Stockage Électrochimique de l'Énergie (RS2E), FR CNRS 3459, France
franck.dolhem@u-picardie.fr

An easy, reliable and cheap access to energy has always been synonym for technological and life quality progresses. The main challenge of our century is to ally energy supply with environmental sustainability.[1] With the ongoing shift from fossil fuels (and its environmental burden) to renewable sources, in transportation (Electric Vehicles or Hybrids) and in energy production, needs in efficient electricity storage devices make rechargeable batteries essential means, not to mention the ever increasing demand induced by the bloom of smart devices (Internet of Things). The accelerating technological growth and worldwide demand for powerful, safer and greener batteries implies to explore new battery chemistries in order to attain the necessary high and green performances.[2] To this respect, the last decade has seen a renewed interest concerning Electroactive Organic Materials (EOMs) due to their intrinsic qualities such as multi-electrons reactions, a wide battery design flexibility, a possible lower environmental impact of the cells, and lower cost.[3–7] Although EOMs could play a major role in the implementation of low-polluting batteries, efforts must be made to develop efficient, safe, and stable high-capacity organic cells. In fact, reports on all-organic metal-ion batteries scarce, due to a critical lack of lithiated organic positive materials.[8]
This contribution aims at reporting recent electrochemical data obtained with crystallized and lithiated organic positive electrode materials and explaining how it is possible to tune their electrochemical activity in order to reach higher potential values (i.e. >3 V vs. Li^+/Li) depending on the molecular assembly and its electrostatic environment. We hope that such findings can pave the way for designing high voltage organic Li-ion batteries in a near future.

References
[1] P. Poizot, F. Dolhem, *Energy Environ. Sci*. **2011**, *4*, 2003-2019.
[2] M. Armand, J.-M. Tarascon, *Nature* **2008**, *451*, 652-657.
[3] F. Cheng, J. Liang, Z. Tao, J. Chen, *Adv. Mater.* **2011**, *23,* 1695-1715.
[4] Z. Song, H. Zhou, *Energy Environ. Sci*. **2013**, *6*, 2280-2301.
[5] P. Poizot, F. Dolhem, J. Gaubicher, S. Renault, *Lithium Process Chemistry: Resources, Extraction, Batteries, and Recycling*, Elsevier, Amsterdam **2015**.
[6] B. Häupler, A. Wild, U. S. Schubert, *Adv. Energy Mater.* **2015**, *5*, 1402034.
[7] Q. Zhao, Y. Lu, J. Chen, *Adv. Mater.* **2017**, *7*, 1601792.
[8] P. Poizot, F. Dolhem, J. Gaubicher, *Curr. Op. Electrochem*. **2018**, *9*, 70-80.

S-Tetrazine as a new redox center for high-performance electrode materials in rechargeable batteries

D. J. Min, S. Y. Park, J. E. Kwon
Research Institute of Advanced Materials (RIAM), Department of Materials Science and Engineering, Seoul National University, Seoul 08826, Republic of Korea
mracle2@snu.ac.kr

With the emerging demand for sustainable and green batteries, organic redox-active molecules have received considerable attention as alternatives to the transition metal oxide-based conventional electrode materials. To date, a lot of organic electrode materials have been reported; but most of them are based on only a few kinds of redox centers including conjugated carbonyls, conducting polymers, and nitroxide radicals. Although these organic materials have demonstrated promising performance particularly in terms of high specific capacity and energy density, they are still inferior to the inorganic electrode materials regarding their low rate performance, high synthesis cost, and fast capacity fading. Therefore, it is imperative to explore a new redox center showing distinctive redox chemistry for developing high-performance organic electrodes.
Herein, we present 1,2,4,5-tetrazine as a new redox center for high-performance electrodes in various types of rechargeable batteries. Because 1,2,4,5-tetrazine, also known as s-tetrazine, has a strong electron deficient character, it typically undergoes a reversible one-electron reduction to form a stable radical anion. First, we synthesized a series of s-tetrazine derivatives and evaluated them as new electrode materials for Li-ion battery.[1] By ex-situ XPS and several electrochemical methods, their peculiar charge/discharge mechanism was fully explored.
Furthermore, a series of polymers bearing s-tetrazines was synthesized and utilized as electrodes in various types of metal-ion batteries. The polymers showed excellent stability over 3000 cycles and superior rate performance. It was found out that their porous nature most likely facilitated metal-ion diffusion which led to high utilization and fast kinetics. Finally, their promising performance as a redox-active host for Li-S battery will also be demonstrated.

References

[1] D. J. Min, F. Miomandre, P. Audebert, J. E. Kwon, S. Y. Park, *ChemSusChem* **2019**, *12*, 503-510.

ABSTRACTS OF ORAL CONTRIBUTIONS

Natural quinones as sustainable battery cathodes

I. K. Ilic, M. Meurer, S. Chaleawlert-umpon, M. Antonietti, C. Liedel
Department of Colloid Chemistry, Max Planck Institute of Colloids and Interfaces, Research Campus Golm, 14476 Potsdam, Germany
clemens.liedel@mpikg.mpg.de

In order to decrease the environmental impact of organic cathode materials, building blocks which can be derived from renewable biomass are especially appealing. Examples for eligible redox active molecules are some flavins and quinones. The latter have the advantage that they might be available in large scale from processing lignin, the most abundant aromatic polymer on earth. One of the most prominent lignin derived small molecules is vanillin, which can be synthesized by copper catalyzed oxidative splitting of lignosulfonates.
It is important to immobilize vanillin for synthesizing stable cathode materials. For this purpose, vanillin may either be polymerized or grafted to a polymeric backbone. In order to keep the process as sustainable as possible, also biopolymeric hosts may be used.
We will present organic cathode materials made of vanillin and similar small molecules, together with biopolymeric linkers. Immobilization approaches as well as electrochemical performance will be discussed, with special focus on the sustainability of the process and material. Being available from biomass, these organic cathodes may be a step towards more benign energy storage materials.

ABSTRACTS OF ORAL CONTRIBUTIONS

Poly(catechol) nanoparticles and their redox activity

K. Pirnat[1,2], N. Casado[2], L. Porcarelli[2], N. Ballard[2], D. Mecerreyes[2]
[1]National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia
[2]POLYMAT, University of the Basque Country UPV/EHU, Joxe Mari Korta Center 20018, Donostia-San Sebastian, Spain
klemen.pirnat@ki.si

Catechols are important compounds in nature and can be found in lignin in wood, as catechin in tea, in plant poison urushiols (poison ivy), as adhesives for underwater organisms and they play important biological roles as catecholamines such as adrenaline and dopamine. In industry, catechol is produced synthetically and is mainly used for pesticides, perfumes and pharmaceuticals. They are also good ligands for metal ions and can be used for waste water treatment for heavy metal removal.[1] Additionally, they show redox activity where they can be reversibly oxidized to *o*-quinones. Due to high theoretical capacity and high redox potential (~3 V vs. Li/Li^+) they are also promising materials for cathodes in Li-organic batteries.[2]
In this work, three different types of poly(catechol) nanoparticles were prepared using polymerization in dispersed media with particle sizes in the range 50-400 nm. They were characterized by DLS, SEM, FTIR, NMR, GPC, TGA and DSC. Their redox activity was tested by CV in aqueous: 0.1 M $HClO_4$ and 0.1 M LiTFSI and nonaqueous electrolyte 0.1 M LiTFSI in acetonitrile. In non-acidic media first cycle shows different behavior due "activation process" and the peaks are shifted to lower potentials due to the formation of lithiated poly (catechols). Generally, the highest redox activity was detected in acidic water electrolyte (Figure 1).

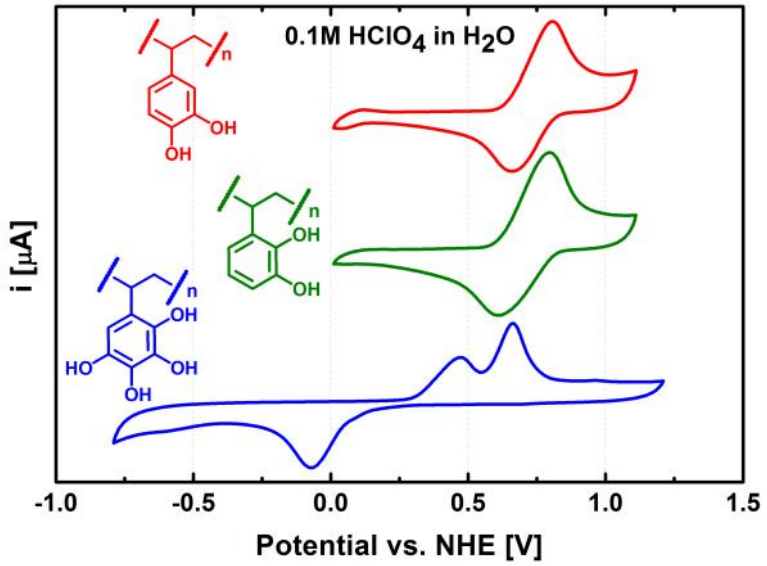


Figure 1: Redox activity of three different poly(catechol) nanoparticles (50 nm) in 0.1 M $HClO_4$ in H_2O.

Acknowledgement
[1] Financial support of the European Research Council by Starting Grant Innovative Polymers for Energy Storage (iPes) 306250
[2] Slovenian research agency (ARRS), research project J2-8167 and public call MS-ERC-FS/2017-002

References
[1] J. Sedó, J. Saiz-Poseu, F. Busqué, D. Ruiz-Molina, *Adv. Mater*. **2013**, *25*, 653-701.
[2] N. Patil, A. Aquil, F. Ouhib, S. Admassie, O. Inganäs, C. Jérôme, C. Detrembleur, *Adv. Mater*. **2017**, *29*, 1703373.

ABSTRACTS OF ORAL CONTRIBUTIONS

The development of a fully printable energy storage technology

A. Wild
Evonik Creavis GmbH, Gebäude 1420 / PB18, Paul-Baumann-Straße 1, 45772 Marl, Germany
andreas.wild@evonik.com

Smart objects are entering our personal and professional lives and offer unprecedented opportunities. Non-toxic, rechargeable and flexible power sources with a tailorable form factor are key elements for such applications. Creavis, the strategic innovation unit of Evonik, is developing materials for organic batteries to fulfill these requirements. The developed materials are fully polymer-based, VOC-free and can be processed via printing technologies. This allows for a seamless integration of the battery into the production process, creating new dimensions of design freedom.

ABSTRACTS OF ORAL CONTRIBUTIONS

Crystallographic change behavior of 2,5-dimethoxy-1,4-benzoquinone during charge and discharge

H. Sano, N. Takeichi, M. Yao, M. Shikano, S. Kuwabata, H. Matsumoto
National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577, Japan
Department of Applied Chemistry, Graduate School of Engineering, Osaka University, Suita, Osaka 565-0871, Japan
hikaru.sano@aist.go.jp

2,5-Dimethoxy-1,4-benzoquinone (DMBQ), which is a low molecule, works as a positive electrode material for lithium-ion batteries according to the two-electron transfer type redox reaction shown in figure (a). The half-cell of DMBQ with a lithium metal counter electrode gives two plateaus at 2.8 V and 2.5 V in its charge-discharge profile, as shown in figure (b). In the XRD measurement of the DMBQ electrode, a pattern derived from the DMBQ crystal was observed in the charged state (lithium-ion de-inserted state), whereas in the discharge state (lithium-ion inserted state) any clear diffraction peak was not observed, as shown in figure ©.[1,2] In the present study, in-situ XRD measurement[3] was carried out and the change in the XRD pattern depending on the depth of charge / discharge was investigated, to clarify the details of the charge-discharge mechanism.
The DMBQ electrode showed a strong diffraction peak derived from the (110) plane of the DMBQ crystal at the higher plateau, and its intensity gradually decreased during the first discharge and finally disappeared. At the lower plateau the DMBQ-derived peak was kept disappeared during the first discharge. During the next charge process, the DMBQ-derived peak was still kept disappeared at the lower plateau; however, gradually recovered at the following higher plateau. It was then considered that the phase where DMBQ crystals lost the long-range order by the lithium-ion insertion increased its volume fraction when the lithium -ions were inserted into the electrode, whereas the phase gradually decreased its volume ratio when the lithium-ions were eliminated from the electrode.

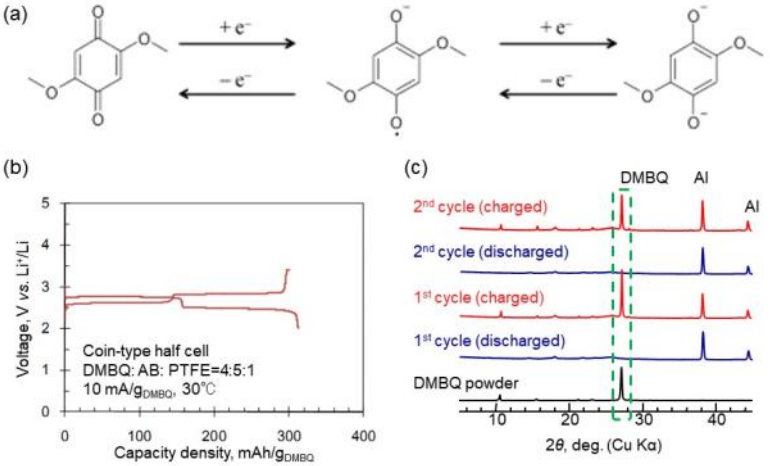


Figure. (a) Redox reaction of DMBQ. (b) First discharge and the following charge curves of the DMBQ-electrode. (c) The XRD patterns of DMBQ powder and DMBQ-electrode after charge-discharge cycles.

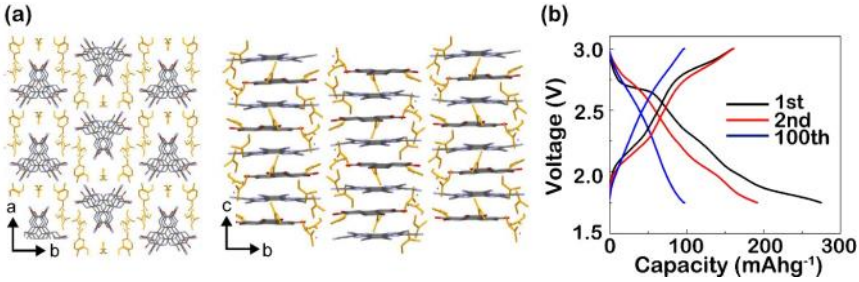
References

[1] M. Yao, H. Senoh, S.-I. Yamazaki, Z. Siroma, T. Sakai, K. Yasuda, *J. Power Sources* **2010**, *195*, 8336-8340.
[2] H. Sano, H. Senoh, M. Yao, H. Sakaebe, T. Kiyobayashi, *Chem. Lett*. **2012**, *41*, 1594-1596.
[3] N. Takeichi et al., Abstract #1845, 222nd ECS Meeting, 7-12 October **2012**, Honolulu, HI.

Cathode performances of porous organic crystals formed by charge-transfer interactions

H. Yoshikawa
Kwansei Gakuin University, Japan
yoshikawah@kwansei.ac.jp

Rechargeable batteries are currently essential power sources for various applications ranging from portable electronics to the emerging large-scale applications. Chemically speaking, almost all developed cathode materials are inorganic ones, which are often costly and not so environmentally benign. To overcome such problems, organic cathode active materials have been considered as promising candidates for promoting new generations of batteries. Among various organic materials, covalent organic frameworks (COFs) have been recently studied as novel organic cathodes since lithium ions can diffuse into their porous structures efficiently.[1] On the other hand, some charge transfer (CT) complexes are also attractive due to their electrochemically active columnar structures with diffusion paths for lithium ions. In this study, we have prepared a novel CT complex (CT-1) composed of hexahydroxytriphenylene (HHTP) as a donor and 1,4,5,8,9,12-hexaazatriphenylene-2,3,6,7,10,11-hexacarbonitrile (HAT-CN) and an acceptor, and its battery performance was examined.
Crystal structure analyses revealed that CT-1 has a pseudo-hexagonal column structure composed of alternate stacking of each component and the voids among columns were filled with solvent molecules, N,N-dimethylformamide (DMF) (Fig. 1(a)). Water adsorption isotherms of CT-1 without solvent molecules suggested that they are porous. Therefore, CT-1 could accommodate lithium ions in the voids during discharge-charge process. Finally, we fabricated an LIB, in which the dried CT-1 was used as cathode active materials. At a current density of 500 mA/g, it exhibited a high discharge capacity of 190 mAh/g during the second cycle (Fig. 1(b)). This capacity was higher than those of only HHTP and HAT-CN. In conclusion, we realized porous organic CT complex batteries with a high capacity. This work was supported by JSPS Core-to-Core Program.



References

[1] S. Wang, Q. Wang, P. Shao, Y. Han, X. Gao, L. Ma, S. Yuan, X. Ma, J. Zhou, X. Feng, B. Wang, *J. Am. Chem. Soc.* **2017**, *139*, 4258-4261.

ABSTRACTS OF ORAL CONTRIBUTIONS

Empowering organic-based negative electrode material through molecular design

L. Fédèle[1-4], O. Ouari[3-4], F. Sauvage[1,2,4], A.Thiam[1,2,4], M. Becuwe[1,2,4]
[1]Laboratoire de Réactivité et Chimie des Solides (LRCS), UMR CNRS 7314, Université de Picardie Jules Verne (UPJV), Amiens, 33 rue Saint-leu, 80039 Amiens, France
[2]Institut de Chimie de Picardie (ICP), FR CNRS 3085, 80039 Amiens, France
[3]Institut de Chimie Radicalaire (ICR), UMR CNRS 7273, Aix Marseille Univ, Marseille 13013, France
[4]Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, 80039 Amiens, France
matthieu.becuwe@u-picardie.fr

Since few years, conjugated organic lithium carboxylates have attracted a particular attention owing to their low cycling potential between 0.7-1.4 V vs Li^+/Li, which paved the way toward the substitution of copper-based current collector by aluminum inducing a reduction of cost and of the embodiment weight. This family presents also several advantages like slight toxicity, can be obtained from eco-friendly process through CO_2 sequestration and structure versatility allowing tuning of the potential. However, performances of this family was still lag behind compare with graphite or LTO.[1]
Different studies have been made over the last three years to optimize conductivity and storage capacity of lithium carboxylate using formulation engineering or crystallization respectively. From our side, we focused our attention on the improvement of the rate capability which was achieved using π–extended aromatic core instead of simple benzene ring. As result we obtained a drastic enhancing of the cycling rate until 2 Li^+/h using a naphthalene or a biphenyl unit as stabilization center.[2,3]
Here, we present the concpetion of a new high-rate cycling material including an anthracene core. The synthesis was realized at gram scale using diaminoanthraquinone as starting compound. This new material presents an unpreceeded reactivity at high rate reaching a capacity of 150 $mAh.g^{-1}$ at 10 C-rate (20 Li^+/h). Additionally, the specific desing of this matertial allows to reduce carbon content additive and so improve electrode capacity, key factor to replace traditional negative electrode material like LTO.

References

[1] M. Armand, S. Grugeon, H. Vezin, S. Laruelle, P. Ribiere, P. Poizot, J.-M. Tarascon, *Nat. Mater*. **2009**, *8*, 120.
[2] L. Fédèle, F. Sauvage, J. Bois, J.-M. Tarascon, M. Becuwe, *J. Electrochem. Soc*. **2014**, *161*, A46-A52.
[3] L. Fédèle, F. Sauvage, S. Gottis, C. Davoisne, E. Salager, J. N. Chotard, M. Becuwe, *Chem. Mater*. **2017**, *29*, 546-554.

ABSTRACTS OF ORAL CONTRIBUTIONS

Molecular electrode materials from nature – design of a green battery

G. John
Department of Chemistry and Center for Discovery and Innovation, The City College of New York, New York, NY 10031, and Ph.D. Program in Chemistry, The Graduate Center of The City University of New York, New York, NY, 10016, USA
gjohn@ccny.cuny.edu

Current lithium ion battery technologies suffer from challenges derived from the eco-toxicity, cost, and energetic inefficiency of contemporary inorganic materials used in these devices. Organic molecules, including polyaromatic carbonyl compounds such as quinones, can be utilized as environmentally friendly alternatives to transition metal oxide-based intercalation cathodes due to their lithium and sodium ion binding capability for LIB/SIB electrodes. Here we demonstrate reversible Na/Li-ion coordination with quinones through the electrochemical reduction of the carbonyl and/or the replacement of hydroxyl group protons with Na/Li. Previous works on stable organic cathodes have mostly focused on the interaction of alkali metal ions with the C=O groups of quinones, which marginalizes the influence of neighboring hydroxyl, amine, and thiol functional groups. Organic molecule-based batteries[1-3] previously exhibited precipitous capacity fading and poor cycling lifetimes due to their solubility in organic electrolytes. We report here that a tetramer (TL) derived from natural henna dye, exhibits stable gravimetric capacities exceeding 100 mAh g^{-1} for over 300 charge/discharge cycles due to coordination with multiple Na/Li ions, as well as the unique stability of metallated salts of TL in electrolytes. The mechanism and chemistry of metal ion binding in the TL were probed using solid-state/solution NMR studies and DFT computations, in conjunction with other spectroscopic methods, reveals that the molecule adopts a nonplanar eight-membered coordination geometry. The new LIB/SIB cathode provides avenues to build fast, stable, high capacity electrodes using organic molecular systems. In addition to the functional utility of these materials, they will be inherently designed to be safe, economic, and environmentally benign. Being constructed from plant derived chemicals to afford smart, throw away batteries to meet the demands of a greener future.

References

[1] D. Larcher, J.-M. Tarascon, *Nat. Chem.* **2015**, *7*, 19-29.
[2] L. Shen, Y. Yu, *Nat. Energy* **2017**, *2*, 836-837.
[3] M. Miroshnikov, K. P. Divya, G. Babu, A. Meiyazhagan, L. M. R. Arava, P. M. Ajayan, G. John, *J. Mater. Chem*. A **2016**, *4*, 12370 - 12386.

ABSTRACTS OF ORAL CONTRIBUTIONS

Understanding superlithitiation of organic electrode materials by evolutionary algorithm DFT calculations

D. Brandell[1], S. Renault[2], R. Pereira de Carvalho[3], C. Marchiori[3], C. M. G. Araujo[3]
[1]Department of Chemistry – Ångström Laboratory, Uppsala University, Box 538, 72121 Uppsala, Sweden
[2]ST2E, Institut des Matériaux Jean Rouxel (IMN), 2 Chemin de la Houssinière, 44300 Nantes, France
[3]Department of Physics and Astronomy, Materials Theory Division, Uppsala University, Box 516, 721 20 Uppsala, Sweden

Computational tools striving towards machine learning techniques and artificial intelligence will provide enormous possibilities for materials design in the future, including the tailoring of organic electrode materials. In this presentation, we will highlight how combinations of evolutionary algorithms in combination with DFT calculations and AIMD simulations can be used to predict crystal structures and electrochemical behavior of organic electrode materials which are difficult to assess with conventional experimental techniques. We will focus this study on the so called 'superlithiated' organic electrode compounds,[1] which can reach extreme capacities through mechanisms which remain largely unveiled. Using predicted crystal arrangements, the electronic structures and the voltage profile for the lithiation process are obtained, and are readily compared to experimental data. Molecular level computations and dynamic simulations provide further insights into the evolution of local structures during the lithitation and delithiation processes.

References

[1] S. Renault, V. A. Oltean, C. M. Araujo, A. Grigoriev, K. Edström, D. Brandell, *Chem. Mater.* **2016**, *28*, 1920-1926.

ABSTRACTS OF ORAL CONTRIBUTIONS

Progress in all-organic rechargeable batteries using the anionic cell configuration

P. Poizot[1,2], A. Jouhara[1], N. Dupré[1], D. Guyomard[1], M. Armand[2], F. Dolhem[3]
[1]Institut des Matériaux Jean Rouxel (IMN), UMR CNRS 6502, Université de Nantes, 2 rue de la Houssinière, B.P. 32229, 44322 Nantes Cedex 3, France
[2]CIC EnergiGUNE, Alava Technology Park, Albert Einstein 48, 01510, Miñano, Alava, Spain
[3]Laboratoire de Glycochimie, des Antimicrobiens et des Agroressources (LG2A), UMR CNRS 7378, Université de Picardie Jules Verne, 33 rue Saint-Leu, 80039 Amiens Cedex, France
philippe.poizot@cnrs-imn.fr

After years of silence, redox-active organic compounds are re-emerging in the energy storage community bringing with them interesting opportunities such as design flexibility, lightweight, low cost and/or restrained environmental burden. In addition, they can potentially integrate a wide variety of electrochemical device architectures operating both in aqueous or non-aqueous electrolytes. In 10 years, tremendous progress has been made to promote organic compounds in various rechargeable storage devices including the redox flow cell configuration.[1-3] Some of them exhibit attractive electrochemical behaviors such as long-term cycling stability and high-rate capability. Finally, they offer different electrochemical activities including the common reversible cation uptake/release as well as access to anion-inserting process bringing to us another playground in designing organic electrochemical storage systems including the development, in principle, of molecular ion batteries.[4,5]
This contribution aims at reporting recent electrochemical data obtained with crystallized p-type organic materials making the formation of all-organic ClO_4^--ion batteries possible. In particular, novel double-zwitterionic redox-active structures will be presented (including their synthesis routes and the corresponding characterization measurements) for possible application as negative electrode materials.

References

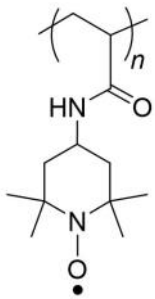
[1] Y. Liang, Z. Tao, J. Chen, *Adv. Energy Mater*. **2012,** *2*, 742-769.
[2] T. Janoschka, M. D. Hager, U. S. Schubert, *Adv. Mater*. **2012**, *24,* 6397-6409.
[3] J. Winsberg, T. Hagemann, T. Janoschka, M. D. Hager, U. S. Schubert, *Angew. Chem. Int. Ed.* **2017**, *56*, 686–711.
[4] M. Yao, H. Sano, H. Ando, T. Kiyobayashi, *Sci. Rep*. **2015**, *5*, 10962.
[5] P. Poizot, F. Dolhem, J. Gaubicher, *Curr. Op. Electrochem*. **2018**, *9*, 70–80.

ABSTRACTS OF ORAL CONTRIBUTIONS

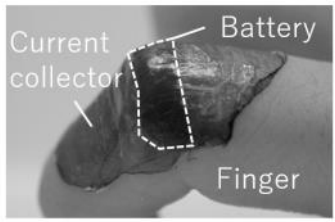
Radical polymer/carbon nanotube hybrids for ultra-thin, stretchable, and solid -state batteries

K. Hatakeyama-Sato, S. Matsumoto, T. Tezuka, H. Nishide, K. Oyaizu
Department of Applied Chemistry, Waseda University, Japan
oyaizu@waseda.jp

Radical polymers, represented by TEMPO-substituted aliphatic polymers, offer high power density, stable voltage, moderate energy density, and flexibility as electrode-active materials, by virtue of their fast redox reactions and facile inter/intramolecular charge propagation.[1,2] We have recently shown that the hybridization of carbon nanotubes (CNTs), having high crystallinity, with radical polymers are synergistically effective to enhance their performances, especially their charge transportability and mechanical properties.[2]
In the presentation, we will report the only 100 nm-thick, free-standing polymer/CNT hybrids for the ultra-thin rechargeable batteries (e.g., total thickness of 1 mm).[3] The successful hybridization firstly enabled the preparation of the intrinsically stretchable batteries (up to 700% length). Further, solid polymer electrolytes and polyviologen derivatives were newly synthesized to obtain the totally solid-state and even transparent rechargeable devices.



Hydrophilic radical polymer



Stretchable battery attached on a finger
(brine as an electrolyte)

References
[1] K. Sato, R. Ichinoi, R. Mizukami, T. Serikawa, Y. Sasaki, J. Lutkenhaus, H. Nishide, K. Oyaizu, *J. Am. Chem. Soc*. **2018**, *140*, 1049-1056.
[2] K. Hatakeyama-Sato, H. Wakamatsu, R. Katagiri, K. Oyaizu, H. Nishide, *Adv. Mater.* **2018**, *30*, 1800900.
[3] K. Hatakeyama-Sato, H. Wakamatsu, K. Yamagishi, T. Fujie, S. Takeoka, K. Oyaizu, H Nishide, *Small* **2019**, *15*, 1805296.

ABSTRACTS OF ORAL CONTRIBUTIONS

Aqueous batteries based on polyimide and prussian blue analogues

S. Kjeldgaard, R. H. Nicolaisen, E. Drazevic, B. Brummerstedt Iversen, A. Bentien
Department of Engineering, Aarhus University, Denmark
Department of Chemistry, Aarhus University, Denmark
bentien@eng.au.dk

Prussian Blue and analogues as cathode[1] and organic polyimides[2] as anode materials are recently being considered as electroactive materials in low-cost and environmentally benign aqueous dry cell batteries.[3-4] Prussian Blue and analogues have the general chemical formula $A_xMFe(CN)_6$, where M is a transition metal (Fe, Zn, Cu, Mn, Co, Ti) and A is typically potassium or sodium. Prussian Blue (M = Fe) and transition metal analogues are stable and insoluble in water, together with the Fe redox activity these materials are well suited as cathode material. As anode different redox active polyimides materials can be synthesized from perylene/naphthalene based monomers and used as anode material.
In the present, we have synthesized and characterized a range of different Prussian Blue analogues and polyimides. For these we have investigated the electrochemical properties in a range of different supporting electrolytes along with battery tests for selected combinations.

References

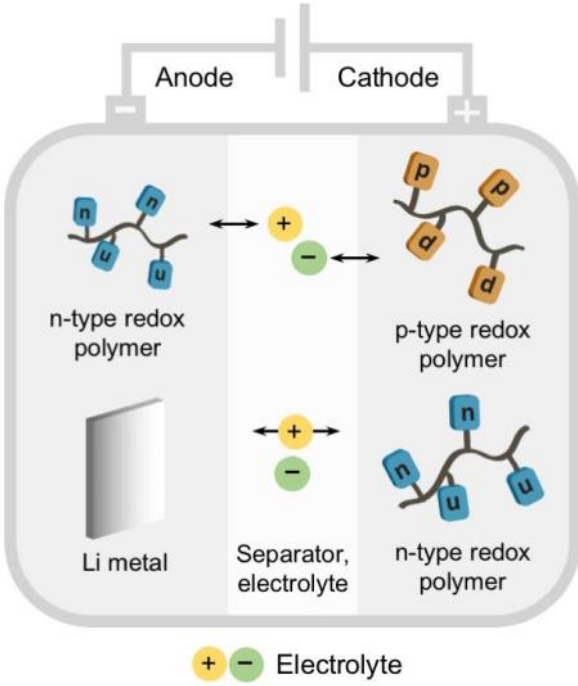
[1] J. Qian, C. Wu, Y. Cao, Z. Ma, Y. Huang, X. Ai, H. Yang, *Adv. Energy Mater.* **2018**, 1702619.
[2] S. Gheytani, Y. Liang, F. Wu, Y. Jing, H. Dong, K. K. Rao, X. Chi, F. Fang, Y. Yao, *Adv. Sci.* **2017**, *4*, 1700465.
[3] E. Dražević, A. S. Andersen, K. Wedege, M. L. Henriksen, M. Hinge, A. Bentien, *J. Power Sources* **2018**, *381*, 94-100.
[4] C. Clausen, E. Dražević, A. S. Andersen, M. L. Henriksen, M. Hinge, A. Bentien, *ACS Appl. Energy Mater.* **2018**, *1*, 243-248.

ABSTRACTS OF ORAL CONTRIBUTIONS

(Hetero)aromatic redox polymers as electrode-active materials for organic batteries

B. Esser
Institute for Organic Chemistry and Freiburg Materials Research Center, University of Freiburg, Germany
besser@oc.uni-freiburg.de

In face of the climate change there is a strong and growing demand for the storage of renewable energies. Reliable electricity storage devices such as batteries and electrochemical capacitors are required.[1] Organic electrode materials have attracted great interest, as they can be prepared from renewable, sustainable or less-limited resources, they are easy to recycle as well as potentially safer and cheaper to produce, leading to a low carbon footprint.[2] A promising class of organic electrode materials are redox polymers – polymers containing groups that can be reversibly reduced or oxidized.[3] In this talk organic redox polymers will be presented containing π-systems as redox-active functionalities.[4-8] The synthesis and electrochemical properties of these polymers will be discussed as well as their application as electrode-active materials in batteries.



References
[1] D. Lindley, *Nature* **2010**, *463*, 18-20.
[2] a) P. Poizot, F. Dolhem, *Energy Environ. Sci*. **2011**, *4*, 2003-2019. b) Y. Liang, Z. Tao, J. Chen, *Adv. Energy Mater*. **2012**, *2*, 742-769. c) Z. Song, H. Zhou, Energy *Environ. Sci.* **2013**, *6*, 2280-2301. d) T. B. Schon, B. T. McAllister, P.-F. Li, D. S. Seferos, *Chem. Soc. Rev*. **2016**, *45*, 6345-6404.
[3] S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka, U. S. Schubert, *Chem. Rev*. **2016**, *116*, 9438-9484.
[4] M. E. Speer, M. Kolek, J. J. Jassoy, J. Heine, M. Winter, P. M. Bieker, B. Esser, *Chem. Commun*. **2015**, *51*, 15261-15264.
[5] M. Kolek, F. Otteny, P. Schmidt, C. Mück-Lichtenfeld, C. Einholz, J. Becking, E. Schleicher, M. Winter, P. Bieker, B. Esser, *Energy Environ. Sci*. **2017**, *10*, 2334-2341.
[6] M. E. Speer, C. Sterzenbach, B. Esser, *ChemPlusChem* **2017**, *82*, 1274-1281.
[7] F. Otteny, M. Kolek, J. Becking, M. Winter, P. Bieker, B. Esser, *Adv. Energy Mater.* **2018**, 1802151.
[8] M. Kolek, F. Otteny, J. Becking, M. Winter, B. Esser, P. Bieker, *Chem. Mater.* **2018**, *30*, 6307-6317.

ABSTRACTS OF ORAL CONTRIBUTIONS

Full organic based aqueous battery with millimeter-thick electrodes

S. Perticarari[1], Y. Pellegrin[2] D. Guyomard[1], F. Odobel[2], P. Poizot[1], J. Gaubicher[1]
[1]IMN, Institut des Matériaux Jean Rouxel, CNRS-Université de Nantes, 2 rue de la Houssiniere, 44322 Nantes Cedex 3, France
[2]CEISAM, Chimie et Interdisciplinarité, Synthèse, Analyse, Modélisation, Université de Nantes, 2, rue de la Houssinière, 44322 Nantes Cedex 3, France
joel.gaubicher@cnrs-imn.fr

Aqueous ionic batteries constitute a novel and promising technology for environmentally friendly grid storage systems as they reduce cost (electrode materials, separator, electrolyte and cell packaging), risk and environmental impact by comparison to other battery technologies, although this is at the expense of energy density.[1] Designing such batteries from inexpensive, abundant, recyclable and non-toxic organic active materials provides a logical step towards improving both the environmental and economic impact of these systems.
Herein, the first ever battery materials that work with simultaneous uptake and release of both cations (Na, Mg) and anions are proposed by designing mixed p -type and n-type "di-block" oligomers.[2] It demonstrates optimal potential, extremely fast kinetics and highly competitive capacity and cyclability in both neutral Na and Mg electrolytes, including ocean water. Through a combination of UV-Vis spectroelectrochemistry, EQCM, and operando synchrotron-XRD a simultaneous cation/anion insertion mechanism was proven and rationalized. The surprisingly fast kinetics of this di-block oligomer allow to attain an unmatched specific capacity of near to 60 mAh/$g_{electrode}$ while entirely devoid of conducting additives, and more than 80 mAh/$g_{electrode}$ with 10% carbon additive.
Based on these findings, full organic cells with millimeter thick electrodes were assembled and tested.[3]These findings may well provide a viable option, thereby promoting the design of cutting-edge, low-cost, rocking-chair dual-ion aqueous batteries.

References

[1] W. Li, J. R. Dahn, D. S. Wainwright, *Science* **1994,** *264*, 1115-1118.
[2] S. Perticarari, Y. Sayed-Ahmad-Baraza, C. Ewels, P. Moreau, D. Guyomard, P. Poizot, F. Odobel, J. Gaubicher, *Adv. Energy Mater.* **2018**, *8,* 1701988.
[3] S. Perticarari, E. Grange, T. Doizy, Y. Pellegrin, A.-J. Fernandez-Ropero, D. Guyomard, P. Poizot, F. Odobel, J. Gaubicher, *Chem. Mater.* **2019**, in press.

ABSTRACTS OF ORAL CONTRIBUTIONS

Development of organic electrode materials for anion-ion batteries

V. Cadiou, L. Merchat, J. Salomon, L. Dubois, D. Guyomard, P. Poizot, T. Gutel
CEA - Univ. Grenoble Alpes, CEA, SYMMES, Conception d'Architecture Moléculaire et Processus Electronique, F-38000 Grenoble, France
lionel.dubois@cea.fr

Organic electroactive compounds such as nitroxide based polymers or carboxylate salts offer a cost-effective and environmental friendly alternative to conventional electrode materials. These products can be prepared from low cost precursors using classical organic and polymer chemistry techniques. Moreover these compounds are easy to recycle or reuse at their end of life. Organic electrode materials can followed n-doped but also p-doped redox mechanisms that enable to imagine new battery configurations (cation-ion, dual-ion or anion-ion). Until now, their use is still challenging due to low cycle life usually related to their high solubility in electrolytes. This work is focused on the development of optimized full organic battery using anion as a shuttle during charge/discharge in order to study their electrochemical performances.
Various polymers based on viologen redox unit were studied as negative electrode materials and the introduction of crosslinker but also the influence of the nature of counter-anion have been investigated. A particular strategy was identified in order to stabilize the specific capacity of polyviologen (PV) along cycling. In parallel, an original and insoluble structure based on lithium dianilinoterephthalate (Li_2DAnT) has been developed and even if some moderate electrochemical performances have been obtained, this development demonstrates for the first time the interest of terephthalate backbone to suppress the dissolution of p-doped organic materials.
The formulation of organic electrodes using PV, Li_2DAnt and polynitroxydes (PTMA) based composites were optimized for screen printing process and several full organic batteries have been assembled and tested in anion-ion configuration. These results pave the way for the development of metal-free battery with high electrochemical performances.

References

[1] P. Poizot, F. Dolhem, *Energy Environ. Sci*. **2011**, *4,* 2003-2019.
[2] A. Iordache, D. Bresser, S. Solan, M. Retegan, M. Bardet, J. Skrzypski, L. Picard, L. Dubois, T. Gutel, *Adv. Sustain. Syst*. **2017**, 1-10.

ABSTRACTS OF ORAL CONTRIBUTIONS

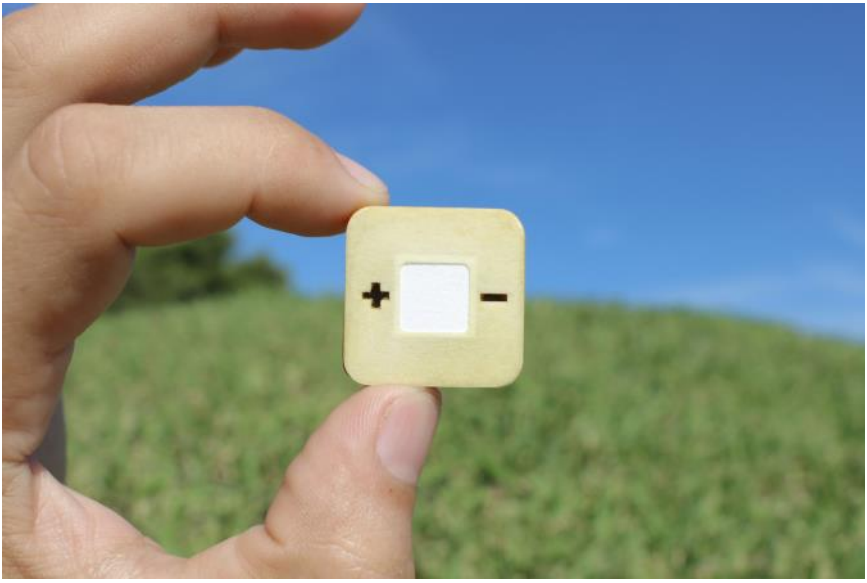
Biodegradable single-use organic batteries for small-sized electronic devices

N. Sabaté [1,2], P. Alday[1], O. Ibrahim[3], E. Kjeang[3], J. P. Esquivel[1]
[1]Instituto de Microelectrónica de Barcelona, IMB-CNM (CSIC), Campus UAB, Spain
[2]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain
[3] Fuel cell Research Lab (FCReL), School of Mechatronic Systems Engineering, Simon Fraser University, Canada
juanpablo.esquivel@csic.es

The vast proliferation of new gadgets and electronic devices in the ICT sector allows foreseeing a significant rise in battery consumption. Generally, these devices are powered with primary cells that are disposed of after depletion. Despite governmental efforts towards reinforcement of recycling policies around the globe, there is a huge number of batteries that are still discarded in an uncontrolled way.

We present a new concept of single-use portable battery specifically made to power small electronic devices that when disposed of, breaks down into simple compounds as a result of the biotic degradative processes of microorganisms present in soils and natural water bodies.[1,2] The battery is made of organic materials such as cellulose, carbon electrodes, beeswax and organic redox species. The power in this device is generated by flowing organic redox pairs through porous electrodes. These redox substances are stored in the paper device and they start flowing by capillarity upon the addition of any available liquid. Once depleted, the device can be disposed with no environmental impact, as it does not contain any metals or harmful substances.

The developed battery is completely aligned with the circular economy principles focusing in the utilization of raw materials that do not cause exhaustion of natural elements, do not require large amounts of energy to be produced, do not produce toxic by-products during their manufacture and feature biodegradability in mild degradation conditions at the end of their life cycle. Such features would thus bypass the need for complex recycling structures and associated investments. In conclusion, this technology radically changes the unsustainable portable battery paradigm, from considering it a harmful waste to a source of materials that can nurture the environment, enrich soil or remove toxins from water beyond the ordinary life cycle of a battery.



References
[1] J. P. Esquivel, P. Alday, O. A. Ibrahim, B. Fernández, E. Kjeang, N. Sabaté, *Adv. Energy Mater.* **2017**, *7*, 1700275.
[2] O. A. Ibrahim, P. Alday, N. Sabaté, J. P. Esquivel, E. Kjeang, J. *Electrochem. Soc.* **2017**, *164*, A2448-A2456.

ABSTRACTS OF ORAL CONTRIBUTIONS

Ultra-low temperature battery based on non-metal design

J. Qin, F. Men, Z. Song, H. Zhan
Department of Chemistry, Wuhan University, Wuhan, 430072, China
zhanhui3620@126.com

Organic electrode material (OEM) earned much attention in the recent years due to their potential high-capacity and much space for further property improvement. However, most OEM greatly suffered from low density and thus-resulted concern on volume specific energy. As light-mass and fluffy is kind of nature of the organics, further processing improvement such as synthesis optimization or architecture optimization cannot sufficiently enhanced the practical tap density of the organics electrode to being comparable to the inorganic cathode in commercial Li-ion battery. Exploring new application and well utilizing the performance advantage of the organics is the key for the further development and potential application of the OEM. Thus, here, we tried to challenge the low temperature limit of the battery and first realized -80 °C battery through a newly non-metal design with organic cathode/anode and ionic-liquid-based electrolyte.

The hybrid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide (EMITFSI), methyl acetate (MA) and acetonitrile (AN) electrolyte successfully reduced the melting point to below -85 °C and maintained an appreciable conductivity until -80 °C. The decent conductivity guaranteed the ion-transfer in electrolyte, and non-intercalation redox mechanism of organic cathode/anode greatly weakened the dependence of redox kinetics on temperature. Thus, the battery working at -80 °C was first achieved without auxiliary heating unit. 79% capacity retention and stable cycling at -80 °C was fulfilled under 1 C-rate. In addition, at -60 °C, the battery still could load more than 70% capacity at 500C and almost 90% capacity at 100C. Owing to the poor-solvation effect and unique quasi-capacitance redox behaviour of the electrodes, ultra-stable cycling of 103.3 mAh g^{-1} capacity after 2000 cycles was obtained at -60 °C. The work not just fills the vacancy of low temperature battery and further push the temperature limit of battery to the aerospace level, it also supplies an effective strategy to conquer the huge SEI and kinetics barrier building with low temperature.

ABSTRACTS OF ORAL CONTRIBUTIONS

High-performance carbonyl electrode materials for rechargeable batteries

J. Chen
Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), Renewable Energy Conversion and Storage Center, College of Chemistry, Nankai University, Tianjin 300071, China
chenabc@nankai.edu.cn

Organic carbonyl electrode materials have shown intriguing interests in rechargeable batteries owing to their environmental friendliness, structural designability, high capacity, and wide abundance. However, common organic carbonyl compounds are easily dissolved in aprotic electrolyte, leading to fast capacity decay and undesired shutting problems with cycling. We here proposed a series of strategies to develop high-performance organic carbonyl electrode materials for rechargeable batteries from four aspects, including molecular engineering, electrode design, electrolyte optimization, and separator modification.[1-3] For example, linking small molecules to polymers and introducing high-polarity functional groups (such as –OM, M=Li, Na, K, etc.) to active molecules are effective to solve the dissolution problem. Developing high-concentration liquid electrolyte or solid-state electrolyte can also enhance the cycling stability of organic carbonyl materials. In addition, by means of the cation-selective property of Nafion, we constructed very stable aqueous Zn–calix[4]quinone batteries (up to 1,000 cycles with a capacity retention of 87% at 500 mA g^{-1}) with Nafion as the separator. Moreover, we developed molecular electrostatic potential to effectively predict the lithiation process of organic electrode materials. These strategies would promote further development of organic carbonyl electrode materials and their practical large-scale applications in the future.

References

[1] Q. Zhao, W. Huang, Z. Luo, L. Liu, Y. Lu, Y. Li, L. Li, J. Hu, H. Ma, J. Chen, *Sci. Adv.* **2018**, *4*, eaao1761.
[2] Z. Luo, L. Liu, J. Ning, K. Lei, Y. Lu, F. Li, J. Chen, *Angew. Chem. Int. Ed.* **2018**, *57*, 9443-9446.
[3] L. Liu, L. Miao, L. Li, F. Li, Y. Lu, Z. Shang, J. Chen, *J. Phys. Chem. Lett.* **2018**, *9*, 3573-3579.

ABSTRACTS OF ORAL CONTRIBUTIONS

Gel electrolytes for organic batteries

A. Lex-Balducci[1,2], S. Muench[1,2], R. Burges[1,2], J. C. Brendel[1,2], M. Jäger[1,2], C. Friebe[1,2], A. Wild[3], U. S. Schubert[1,2]
[1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldstr. 10, 07743 Jena, Germany
[2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany
[3]Evonik Creavis GmbH, Paul-Baumann-Straße 1, 45772 Marl, Germany
a.lex-balducci@uni-jena.de

Since the first report in 2002 by Nakahara *et al.*,[1] organic batteries have been intensively studied, as they feature several advantages compared to current metal-based batteries such as lithium ion batteries. Besides the higher flexibility and lower toxicity due to the use of organic active materials that do not comprise any scarce, harmful or toxic metals, organic batteries offer the possibility to be produced in a cost-efficient way by applying manufacturing techniques such as roll-to-roll processing or printing. In the last years, a lot of research work has been dedicated to the development of new active materials. However, the work on electrolyte systems specially developed for organic batteries is sparse. This is not only the case for liquid systems, but in particular for polymer electrolytes – the system of choice for printable organic batteries. There are just a few reports on polymer electrolytes for organic batteries in literature so far; however, none of the descripted systems is printable.
In this contribution, we present the first example of a printable gel polymer electrolyte especially designed for solid state all-organic batteries.[2] The developed electrolyte formulation is a viscous paste, which can be directly casted on the electrodes and subsequently polymerized by UV-polymerization. The formulation comprises a mixture of methacrylate-based monomers including a cross-linking agent, a photo initiator, a nano-filler for the adjustment of the viscosity and an ionic liquid serving as solvent. After the UV-polymerization the ionic liquid serves as conductive salt in the resulting flexible, mechanically stable polymer electrolyte film. Therefore, this system offers the advantage that no post-treatment step, e.g., evaporation of solvent, is necessary. The polymer electrolyte, which has a high ionic conductivity at room temperature (in the range of 10^{-4} S cm^{-1}), was successfully applied as electrolyte and separator in all-organic batteries.

References

[1] K. Nakahara, S. Iwasa, M. Satoh, Y. Morioka, J. Iriyama, M. Suguro, E. Hasegawa, *Chem. Phys. Lett.* **2002**, *359*, 351-354.
[2] S. Muench, R. Burges, A. Lex-Balducci, J. C. Brendel, M. Jäger, C. Friebe, A. Wild, U. S. Schubert, submitted.

ABSTRACTS OF ORAL CONTRIBUTIONS

The influence of the electrolyte composition on the electrochemical performance of organic batteries

P. Gerlach[1,2], A. Lex-Balducci[2,3], U. S. Schubert[2,3], A. Balducci[1,2]
[1]Institute for Technical Chemistry and Environmental Chemistry, Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany
[2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany
[3]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldstr. 10, 07743 Jena, Germany
andrea.balducci@uni-jena.de

Organic radical polymers (ORPs) combine a favourable redox chemistry with favourable kinetics for energy storage.[1] Due to these properties, and thanks to their affordable price, the interest on the use of these polymers for the realization of metal-free batteries constantly increased in the last years. Several types of polymers have been proposed and, among them, the poly(2,2,6,6-tetramethylpiperidinyl-N-oxymethacrylate) (PTMA), which bears a TEMPO group in every repeating unit, has been one of the most investigated.[1] Several studies showed that this ORP, which was firstly reported by Nakahara et al. and feature a theoretical capacity of 111 mAh/g, displays high rate capabilities and good cycling stability when used in combination with conventional lithium-ion battery (LIBs) electrolytes such as 1 M $LiPF_6$ EC/DEC. These latter electrolytes have been considered because they are a state-of-the-art of LIB, which is an established technology. Nevertheless, it is important to notice that the use of lithium salts is not mandatory for the realization of ORP-based batteries, and also electrolytes not containing metal salts could be used. These “alternative” electrolytes would contribute to the realization of (completely) metal-free systems.
In this work, we investigated the influence of “metal-free” electrolytes on the performance of PTMA based electrodes. Two aspects have been particularly addressed: (1) the presence/absence of the solvent and (2) the salt concentration of the electrolyte. The results of these studies clearly indicate that the nature of the electrolyte as well as the electrolyte concentration has a strong influence on the capacity, capacity retention and especially self-discharge of PTMA-based electrodes.[2,3]

References

[1] S. Muench, A. Wild, C. Friebe, B. Haupler, T. Janoschka, U.S. Schubert, *Chem. Rev.* **2016**, *116*, 9438–9484.
[2] P. Gerlach, R. Burges, A. Lex-Balducci, U. S. Schubert, A. Balducci, *J. Power Sources*, **2018**, *405*, 142-149.
[3] P. Gerlach, R. Burges, A. Lex-Balducci, U. S. Schubert, A. Balducci, *Electrochim. Acta* **2019**, *306*, 610-616.

ABSTRACTS OF ORAL CONTRIBUTIONS

Design for long cycle-life quinone-type active materials by oligomerization

M. Yao, M. Kato, H. Ando, T. Kiyobayashi, N. Takeichi
National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577, Japan
m.yao@aist.go.jp

As a candidate category of minor-metal free electrode materials for use in rechargeable lithium batteries, we have focused on a series of low-molecular-weight quinone derivatives.[1] These compounds have high theoretical capacity based on their multi-electron transfer reactions; however, they often show poor cycle-stabilities. One of the reasons for the capacity fade is believed to be the dissolution of redox active molecules into the electrolyte solution.
To suppress the dissolution, we found that the oligomerization of the redox active units is an effective way. For example, in the case of the anthraquinone (AQ) derivatives, a fused molecule or acetylene-unit-connected oligomers, which have a lower solubility, exhibits a longer cycle-life than the AQ monomer.[2] A similar result was also observed for the naphthazarin (5,8-dihydroxy-1,4-naphthoquinone) derivatives exhibiting high discharge capacities of about 400 mAh/g[3] as shown in the figure below.
A quantum chemistry calculation revealed that the intermolecular binding energy becomes a few times higher by the oligomerization than that of the monomer. The estimated binding energy values (80-120 kJ/mol) for the oligomers are comparable to the level of the covalent bonding (100-300 kJ/mol), which would be beneficial to suppress the dissolution of the organic active materials into the electrolyte solutions.
Our finding in this study will be a guide to design a novel organic compound showing a high capacity and good cycling performance.

References

[1] M. Yao, H. Senoh, S. Yamazaki, Z. Siroma, T. Sakai, K. Yasuda, *J. Power Sources* **2010**, *195*, 8336-8340.
[2] M. Yao, S. Yamazaki, H. Senoh, T. Sakai, T. Kiyobayashi, *Mater. Sci. Eng. B* **2012**, *177*, 483-487.
[3] M. Yao, H. Ando, T. Kiyobayashi, N. Takeichi, The 57th Battery Symposium in Japan, **2016**, #3A09.

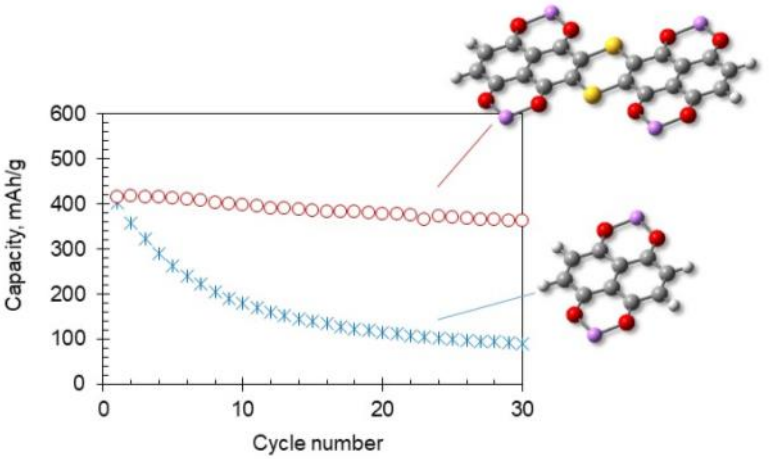


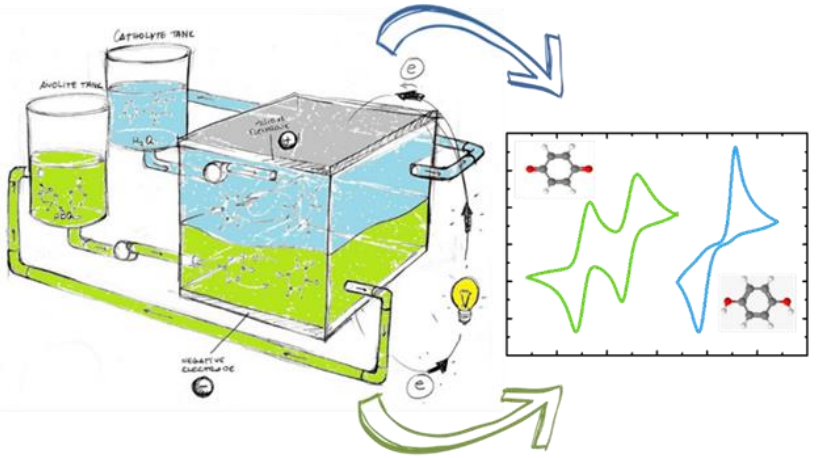
Fig. Cycle-life performance of the electrodes using the Li-salt of naphthazarin monomer (∗) and the dithiin-fused dimer (○).

ABSTRACTS OF ORAL CONTRIBUTIONS

Metal-free and membrane-free redox flow batteries by using immiscible electrolytes based on organic redox molecules

R. Marcilla
Electrochemical Processes Unit, IMDEA Energy Institute, Avda. Ramón de la Sagra 3, 28935 Móstoles, Spain
rebeca.marcilla@imdea.org

Wide-spread implementation of conventional RFBs is limited by some obstacles related to low abundance, toxicity and high cost of vanadium redox compounds, and the poor-performing and expensive ion exchange membranes. Excepting polymer-based RFB[1] where crossover can be mitigated with an inexpensive size-exclusion separator, most RFB require an ion-exchange membrane to prevent the crossover of active species. This key element can account for more than 30 % of the cost of the battery[2] and may limit the long-term battery performance due to unavoidable cross-contamination and insufficient mechanical, chemical and electrochemical stability.
Here, I present an innovative concept of Membrane-Free Battery which proposes to eliminate any separator or membrane by using immiscible redox electrolytes[3]. Moreover, the vanadium redox species are replaced by cheap and abundant organic redox molecules that can be specifically designed to exhibit high solubility, adequate redox potentials and suitable partition coefficient between the two immiscible phases. It will be demonstrated that this disruptive technology is hugely versatile with respect to the type of organic redox species as well as the nature of immiscible electrolytes forming the biphasic system. We will discuss the electrochemical performance of Membrane Free batteries based on aqueous/non-aqueous immiscible electrolytes[4] but also a Total Aqueous Membrane-free Battery in which the two phases are aqueous[5], which brings some advantages in terms of cost, environmental issues and battery performance. New challenges such as the inherent selfdischarge in the liquid-liquid interface and future opportunities of this innovative technology will be also discussed.



References
[1] a) G. Nagarjuna, J. Hui, K. J. Cheng, T. Lichtenstein, M. Shen, J. S. Moore, J. Rodríguez-Lopez, *J. Am. Chem. Soc*. **2014**, *136*, 16309-16316. b) T. Janoschka, N. Martin, U. Martin, C. Friebe, S. Morgenstern, H. Hiller, M. D. Hager, U. S. Schubert, *Nature* **2015**, *527*, 78-81.
[2] M. Zhang, M. Moore, J. S. Watson, T. A. Zawodzinski, R. M. Counce, *J. Electrochem. Soc.* **2012**, *159*, A1183-A1188.
[3] P. Navalpotro, J. Palma, M. Anderson, R. Marcilla, *Angew. Chem. Int. Ed.* **2017**, *56*, 12460-12465.
[4] P. Navalpotro, N. Sierra, C. Trujillo, I. Montes, J. Palma, R. Marcilla, *ACS Appl. Mater. Interfaces* **2018**, *10*, 41246-41256.
[5] P. Navalpotro, C. Neves, J. Palma, M. G. Freire, J. A. P. Coutinho, R. Marcilla, *Adv. Sci.* **2018**, *5*, 1800576.

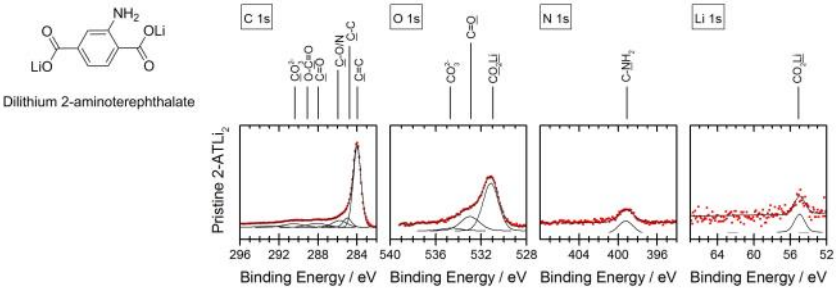
Acknowledgments
MFreeB project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 726217).

ABSTRACTS OF ORAL CONTRIBUTIONS

Further investigations of the electrode/electrolyte interface of organic electrode materials for Li-ion batteries

A. Naylor[1], D. Brandell[1], S. Renault[2]
[1]Department of Chemistry - Ångström Laboratory, Uppsala University, Uppsala Sweden
[2] IMN, University of Nantes, Nantes, France
steven.renault@cnrs-imn.fr

The formation of a solid electrolyte interphase (SEI) is well-known and characterized for inorganic LiB materials. However, it has been scarcely investigated for organic electrode materials (OEMs). It is speculated that the formation of a less stable SEI layer for OEMs and its evolution during battery cycling could be at the origin of several issues for these batteries such as decreasing capacity or loss of material during cycling. One of the main reasons for these scarce studies is due to the difficulty to distinguish the OEMs contribution from the decomposition materials coming from either OEMs or electrolyte, which are all composed of the same elements (C, H, O, Li).[1]
We recently investigated the electrochemical behaviour of dilithium 2-aminoterephthalate, a nitrogen-containing OEM[2] Further investigations on this material, its complexation ability and a battery design/electrode formulation free of any other sources of nitrogen permitted us to perform a thorough X-ray photoelectron spectroscopy (XPS) study. Using N 1s core level peaks as a marker, we were able to discriminate the signals of different elements depending of their origin. The results will be presented with the aim to improve the comprehension of some electrochemical features of OEMs.



References

[1] V. A. Oltean, B. Philippe, S. Renault, R. F. Duarte, H. Rensmo, D. Brandell, *Chem. Mater*. **2016**, *28*, 8742-8751.
[2] S. Renault, V. A. Oltean, M. Ebadi, K. Edström, D. Brandell, *Solid State Ionics* **2017**, *307*, 1-5.

ABSTRACTS OF ORAL CONTRIBUTIONS

Insight into solid-state electrochemistry of bi-redox organic battery materials

A. E. Lakraychi, A. Vlad
Institute of Condensed Mater and Nanosciences, Université Catholique de Louvain, Belgium
alae.lakraychi@uclouvain.be

Carbonyl compounds have been clearly recognized as the most promising electroactive materials for organic batteries.[1] In this context, molecular engineering has played a big part in improving the electrochemical performances in terms of tuning the potential[2] and preventing the solubility.[3] However, these improvements partially penalize the gravimetric capacities, and the exact origin of the redox potential shift as well as redox mechanism are still matter of debates. In this work, we will try to address both issues. First, we will detail on the electrochemistry of aromatic and heterocyclic dicarboxylate isomers. This study comprehends (i) the effect of N-heteroatom on the potential of the dicarboxylates, with a direct correlation between the potential and the ^{13}C-chemical and vibration frequency shift of the carbonyl and (ii) the redox mechanism unveiling the structural requirements that dictates the electrochemical activity of either dicarboxylate or pyrazine redox units. Secondly, we will show how by using coordination chemistry, new multi-electron materials with bi-polar redox activity can be designed. The materials can deliver capacities in excess of 200 mAh.g^{-1} at an average working (reduction) potential of 3 V (vs. Li^+/Li^0).

References

[1] a) P. Poizot, F. Dolhem, *Energy Environ Sci*. **2011**, *4*, 2003-2019.
b) S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka, U. S. Schubert, *Chem. Rev*. **2016**, *116*, 9438-9484. c) Y. Liang, Y. Yao, *Joule*. **2018**, *2*, 1690-1706.
[2] a) A. E. Lakraychi, E. Deunf, K. Fahsi, P. Jimenez, J.-P. Bonnet, F. Djedaini-Pilard, M. Bécuwe, P. Poizot, F. Dolhem, *J. Mater. Chem. A* **2018,** *6*, 19182-19189. b) A. Jouhara, N. Dupré, A.-C. Gaillot, D. Guyomard, F. Dolhem, P. Poizot, *Nat. Comm*. **2018**, *9*, 4401.
[3] L. Sieuw, A. Jouhara, E. Quarez, C. Auger, J.-F. Gohy, P. Poizot, A. Vlad, *Chem. Sci*. **2019**, *10*, 418-426.

ABSTRACTS OF ORAL CONTRIBUTIONS

Redox-active polymer based nano-objects via polymerization induced self-assembly

F. Boujioui, J.-F. Gohy
Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium.
jean-francois.gohy@uclouvain.be

Flow-assisted electrochemical systems (FAES) are receiving increasing interest because of their application in various systems including redox flow battery (RFB), electrochemical flow capacitor (EFC) and semi-solid flow battery (SSFB). For this type of electrochemical systems, the active species are stored in solution in external tanks and pumped through the main cell to fuel it continuously, thereby generating the energy. While the energy density is related to the size of the tanks, the power density is determined by the composition of electrodes. The suspension electrodes are called catholytes or anolytes and are composed between 5 and 20 wt. % of active storing material, contrary to the electrode films used in batteries for which the composition is greater than 80 wt. %. Among the different materials used for the preparation of suspension electrodes, redox-active polymers are receiving special interest because their properties can be easily tailored by macromolecular engineering. For example, their solubility can be tuned in various solvents by co-polymerizing with the adequate monomers. Their molar masses, molar masses distribution as well as their architectures (i.e. linear, branched, statistical, block copolymers, etc.) can be easily tuned provided that controlled or living polymerization techniques are used for their synthesis. Poly(2,2,6,6-tetramethylpiperidinyloxy-4-yl-methacrylate) (PTMA) is indeed considered as an excellent redox-active polymer for application in FAES.[1]
One of the main challenges related to redox-active polymer-based electrodes remains the relatively low concentration of redox-active material that can be dissolved while keeping a viscosity sufficiently low to allow the pumping of the liquid electrode in the main electrochemical cell. Decreasing the molar mass of the polymer is not a valid option since the electroactive polymer should not pass through the semi-permeable membrane located in the main electrochemical cell. One way to allow the dispersion of a high amount of electroactive polymer while not reaching a too high viscosity consists in tethering the redox-active polymer chains in a micellar design. Basically, the redox-active polymer chains could be incorporated into two different compartment of the micellar cargo: the micellar core or the micellar corona.
In this respect, we have designed micellar nano-objects comprising PTMA coronal chains tethered onto a polystyrene (PS) core. Those objects were synthesized from PTMA-b-PS diblock copolymers containing a major PTMA block dissolved in carbonate solvents that are selective solvents for the PTMA

blocks.[2] The accordingly obtained micelles were successfully tested as catholytes in RFB.[3] Such a design presents the advantage to allow a good accessibility of the electroactive PTMA chains for redox reaction since they are located in the micellar corona but the disadvantage to be limited to organic solvents for the preparation of the liquid electrode since both PTMA and PS are hydrophobic groups.

Aqueous micellar catholytes could however be obtained from amphiphilic block copolymer containing a water-soluble hydrophilic block and a hydrophobic PTMA block. In aqueous medium, such a copolymer is expected to form micellar nano-objects containing a PTMA core and a hydrophilic polymer corona. In order to maximize the amount of PTMA in the system, the composition of our copolymers will be adjusted to target cylindrical micelles rather than spherical ones. Practically, our attention is focused on the so-called polymerization induced self-assembly (PISA) method. This method has indeed emerged as a promising alternative to classical water-based polymerization techniques since it is surfactants-free (the formed copolymer plays indeed the role of surfactant) and it leads to the formation of the micellar nano-objects directly during the synthetic process of the copolymer. The strategy developed in the present contribution is to synthesize directly PTMA based nano-objects in suspension in aqueous medium by copolymerizing it with a hydrophilic polymer block using a PISA process. Herein, we report the RAFT polymerization induced self-assembly of the 2,2,6,6-tetramethylpiperidin-4-yl methacrylate (TMPM) monomer which is the precursor of the PTMA. Two types of water-soluble macro-CTAs are synthesized, i.e. the thermo-responsive poly[oligo(ethylene glycol) methyl ether methacrylate] (POEGMA) and the cationic poly[(4-methacryloyloxy)-2,2,6,6-tetramethylpiperidinium chloride] (PTMPM+Cl-). This PISA process leads to the formation of micellar nano-objects with a PTMPM core and either a POEGMA or a $PTMPM^{+}Cl^{-}$ corona. After the oxidation step to transform PTMPM into PTMA, the redox properties of redox-active polymer based nano-objects are confirmed through cyclic voltammetry measurements.

References

[1] (a) J. Winsberg, T. Hagemann, T. Janoschka, M. D. Hager, U. S. Schubert, *Angew. Chem. Int. Ed*., **2017**, *56*, 686-711. (b) J. Winsberg, T. Janoschka, S. Morgenstern, T. Hagemann, S. Muench, G. Hauffman, J. F. Gohy, M. D. Hager, U. S. Schubert, *Adv. Mater*. **2016**, *28*, 2238-2243. (c) T. Janoschka, N. Martin, U. Martin, C. Friebe, S. Morgenstern, H. Hiller, M. D. Hager, U. S. Schubert, *Nature* **2015**, *527*, 78-81.

[2] G. Hauffman, Q. Maguin, J. P. Bourgeois, A. Vlad, J. F. Gohy, *Macromol. Rapid Commun.* **2014**, *35*, 228-233.

[3] J. Winsberg, S. Muench, T. Hagemann, S. Morgenstern, T. Janoschka, M. Billing, F. H. Schacher, G. Hauffman, J. F. Gohy, S. Hoeppener, M. D. Hager, U. S. Schubert, *Polym. Chem*. **2016**, *7,* 1711-1718.

EuChemS

European Chemical Society

EuChemS, the European Chemical Society, aims to nurture a platform for scientific discussion and to provide a single, unbiased European voice on key policy issues in chemistry and related fields.

Representing more than 160,000 chemists from more than 40 Member Societies and other chemistry related organisations, EuChemS relies on a unique network of active researchers involved in all the fields of chemistry. Through this network, EuChemS organises several specialised academic conferences as well as the biannual EuChemS Chemistry Congress, the European congress of chemical sciences. EuChemS also promotes the role and image of the chemical sciences among the general public and policy-makers through social media, newsletters and through the organisation of conferences and workshops open to the society.

Through the promotion of chemistry and by providing expert and scientific advice, EuChemS aims to take part of the solution to today´s major societal challenges.

For more information about the European Chemical Society (EuChemS), please visit www.euchems.eu or contact us at:

EuChemS aisbl
Rue du Trône 62
1050 - Brussels
Belgium

Phone: +32 2289 25 67 | +32 2289 26 90

Email: secretariat@euchems.eu

http://on.fb.me/1B8Qa0n

https://twitter.com/EuCheMS

List of Poster Presentations

LIST OF POSTER PRESENTATIONS

P 01	Itaconic acid as a building block for sustainable solid polymer electrolytes *Dr. Muhammad Abdelhamid* *Uppsala University, Uppsala (SE)*
P 02	Synthesis of redox active quinoid polymers and application to electrode-active materials for organic secondary batteries *Tomoki Akahane* *Waseda University, Tokyo (JP)*
P 03	The proton trap - a new route to organic energy storage *Lisa Åkerlund* *Uppsala University, Uppsala (SE)*
P 04	Organic cathode materials for rechargeable Mg batteries *Dr. Jan Bitenc* *National Institute of Chemistry, Ljubljana (SI)*
P 05	Isoindoline nitroxide derived high-voltage cathode materials *Dr. James P. Blinco* *Queensland University of Technology, Brisbane (AU)*
P 06	Sodium conducting hybrid solid polymer electrolytes for energy storage devices *Johannes Buchheim* *Friedrich Schiller University Jena, Jena (DE)*
P 07	“Water-in-ionic liquids” promoted utilization of redox-active organic materials for flow batteries *Dr. Ruiyong Chen* *Saarland University, Saarbrücken (DE)*

LIST OF POSTER PRESENTATIONS

P 08	Natural organic molecular based hierarchically porous carbon for enhanced supercapacitive performance *Min Sung Choi* *SungKyunKwan University, Suwon (KR)*
P 09	Understanding the structure and electrochemistry of dicarboxylate electrodes from first-principles theory *Rodrigo de Carvalho* *Uppsala University, Uppsala (SE)*
P 10	Phenothiazine and dibenzocyclooctatetraene-based polymers as electrode materials for organic batteries *Gauthier Desmaizieres* *University of Freiburg, Freiburg (DE)*
P 11	Development of high solubility catholytes for organic aqueous redox flow batteries *Dr. Emil Dražević* *Aarhus University, Aarhus (DK)*
P 12	Assessing crossover in redox flow batteries: a novel electrochemical method *Dr. Filippo Fenini* *Aarhus University, Aarhus (DK)*
P 13	The influence of the salt concentration on the electrochemical performance of electrodes for polymeric batteries *Patrick Gerlach* *Friedrich Schiller University Jena, Jena (DE)*
P 14	Characterizing the ionic conductivity of solid polymer electrolytes using distribution of relaxation times *Markus Hahn* *University of Bayreuth, Bayreuth (DE)*

LIST OF POSTER PRESENTATIONS

P 15	Solar light rechargeable redox-flow batteries *Dr. Christoph Haisch* *DECHEMA-Forschungsinstitut, Frankfurt am Main (DE)*
P 16	One-pot synthesis of multidimensional structured 3D nanohybrid material for high performance energy storage *Mingyu Jung* *SungKyunKwan University, Suwon (KR)*
P 17	Supercapacitors employing oak-wood-derived porous carbons impregnated with quinones *Yuto Katsuyama* *Tohoku University, Sendai (JP)*
P 18	Exploiting nicotinamide cofactor from natural energy transduction as bio-inspired lithium-ion batteries *Jihyeon Kim* *Seoul National University, Seoul (KR)*
P 19	Evaluating organic redox reactants for biodegradable primary batteries for small electronic devices *Dr. Erik Kjeang* *Simon Fraser University, Burnaby (CA)*
P 20	Polyimide/copper hexacyanoferrate - a low cost battery for large-scale energy storage *Solveig Kjeldgaard* *Aarhus University, Aarhus (DK)*
P 21	Dissolution/re-deposition processes in poly (vinylphenothiazine)-based Li–organic batteries *Martin Kolek* *University of Münster, Münster (DE)*

LIST OF POSTER PRESENTATIONS

LIST OF POSTER PRESENTATIONS

P 29	A novel binder-free cathode based on electro-polymerized conductive polymer for Li-S batteries *Dr. Shilin Mei* *Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin (DE)*
P 30	Structure-property relations of quinone-based active materials for redox flow batteries *Prof. Dr. Doreen Mollenhauer* *Justus-Liebig University Giessen, Giessen (DE)*
P 31	Printable gel polymer electrolyte for all-organic batteries *Simon Münch* *Friedrich Schiller University Jena, Jena (DE)*
P 32	Electronically tunable redox-active organic mediators *Dr. Alex Murray* *University of Kent, Canterbury (GB)*
P 33	Organic secondary battery using neutral aqueous electrolyte solution *Yuto Nakagawa* *University of Tsukuba, Tennōdai (JP)*
P 34	Aqueous sodium-ion battery with a naphthalene tetra-carboxylic diimide (NDI) electrode embedded in a metal-organic framework (MOF) *Dr. Kosuke Nakamoto* *Kyushu University, Fukuoka (JP)*
P 35	Eco-friendly cellulose-chitosan hydrogel batteries *Marina Navarro Segarra* *Institute of Microelectronics of Barcelona IMB-CNM, Barcelona (ES)*

LIST OF POSTER PRESENTATIONS

P 36	Asymmetric aqueous Li-S capacitor with bisalt soaked poly acrylic acid gel electrolyte and n-doped activated carbon-sulfur(NAC-S) *Jae Min Park* *SungKyunKwan University, Suwon (KR)*
P 37	Macromolecular engineering of redox-active polymers bearing catechol pendants: promising paradigm towards high-performance organic batteries *Dr. Nagaraj Patil* *IMDEA Energy Institute, Madrid (ES)*
P 38	Structural variation of poly(vinylphenothiazine)-based cathode-active materials for rechargeable Li/organic batteries *Verena Perner* *University of Münster, Münster (DE)*
P 39	Quinone based organic composite electrodes for sodium-ion batteries *Dr. Engelbert Portenkirchner* *University Innsbruck, Innsbruck (AT)*
P 40	Crosslinked polymer electrolytes from imidazolium-based ionic liquid monomers *Eike Thomas Röchow* *Leibniz-Institut für Polymerforschung Dresden e.V., Dresden (DE)*
P 41	Reduced graphene oxide /poly (pyrrole-co-thiophene) composite framework for energy storage in supercapacitors *Prof. Dr. Anwar-ul-Haq Ali Shah* *University of Peshawar, Peshawar (PK)*

LIST OF POSTER PRESENTATIONS

P 42	Porphyrinoids as cathode materials for high-performance lithium-ion batteries *Shirin Shakouri* *Karlsruher Institute of Technology, Karlsruhe (DE)*
P 43	Binder- and conducting additive-free organic electrode materials - post-deposition polymerization of conducting redox oligomers *Christian Strietzel* *Uppsala University, Uppsala (SE)*
P 44	Methylphenothiazine-based polymers as cathode-active materials for organic batteries *Gauthier Studer* *Albert-Ludwigs-University of Freiburg, Freiburg (DE)*
P 45	Polyimide/multiwalled carbon nanotubes nanocomposite as cathode materials for post Li metal-organic batteries *Dr. John F. Vélez-Santa* *National Institute of Chemistry, Ljubljana (SI)*
P 46	Investigating an all-organic battery using polyisothianaphthene as a redox-active bipolar electrode material *Prof. Dr. Fu-Ming Wang* *National Taiwan University of Science and Technology, Taipei City (TW)*
P 47	Side chain quinone redox reaction effects on conductivity of quinone-PEDOT based conducting redox polymer *Huan Wang* *Uppsala University, Uppsala (SE)*

LIST OF POSTER PRESENTATIONS

P 48	Anthraquinone/carbon paper composite electrodes for organic sodium ion batteries *Daniel Werner* *University Innsbruck, Innsbruck (AT)*
P 49	Post-polymerization modification for the synthesis of radical containing polymers *Wenwen Xue* *Karlsruher Institute of Technology, Karlsruhe (DE)*
P 50	Energy system simulation of redox flow batteries in different applications in the low-voltage grid *Christina Zugschwert* *University of Applied Sciences Landshut, Landshut (DE)*

Abstracts of Poster Presentations

ABSTRACTS OF POSTER PRESENTATIONS

P 01: Itaconic acid as a building block for sustainable solid polymer electrolytes

M. E. Abdelhamid[1], S. Renault[2], J. Mindemark[1], D. Brandell[1]
[1]Department of Chemistry - Ångström Laboratory, Uppsala University, Uppsala, Sweden
[2]Institut des Matériaux Jean Rouxel (IMN), University of Nantes, Nantes, France
muhammad.abdelhamid@kemi.uu.se

Nowadays, most of energy storage solutions for mobile applications are based on Li-ion technology since its commercialisation in the early 1990s. This is due to its unsurpassed gravimetric and volumetric energy density. However, the production of Li-ion batteries (LiBs) requires large amount of non-renewable resources (e.g. inorganic ores and petroleum-based materials), energy, and toxic chemicals, which raise concerns about their environmental impact and resource depletion effect.[1] As a result, research on organic battery electrode materials for organic Li-ion batteries (OLiBs) has grown with significant results.[2]
Although, the focus on the organic electrode materials, fewer studies targeted the development of bio-derived electrolytes designed for OLiBs. Given that most of the LiBs polymer electrolytes are derived from petroleum products, it is necessary to develop polymers that are sourced from renewable resources (e.g. biomass) to reduce the fossil fuel print in and achieve sustainable all-organic batteries. Itaconic acid is an example of a compound that could serve as a versatile green building block for electrolytes due to its abundance and ease of extraction from natural carbohydrates.[3] Here, we present the synthesis and characterisation of a novel polymer electrolyte based on itaconic acid as well as performance comparison with other standard polymer electrolytes.

References

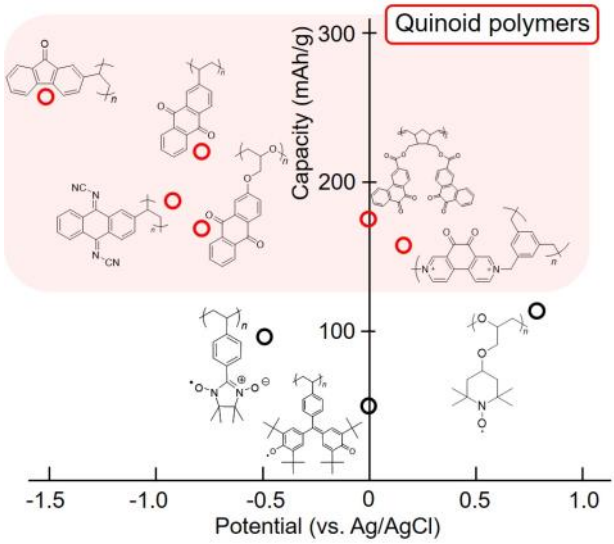
[1] C. J. Barnhart, S. M. Benson, *Energy Environ. Sci.* **2013**, *6*, 1083-1092.
[2] P. Poizot, F. Dolhem, J. Gaubicher, *Curr. Opin. Electrochem.* **2018**, *9*, 70-80.
[3] http://www.nrel.gov/docs/fy04osti/35523.pdf. 2016-04-09.

ABSTRACTS OF POSTER PRESENTATIONS

P 02: Synthesis of redox active quinoid polymers and application to electrode-active materials for organic secondary batteries

T. Akahane, C. Go, K. Hatakeyama-Sato, K. Oyaizu
Department of Applied Chemistry, Waseda University, Tokyo 169-8555, Japan
tomoki.akahane@akane.waseda.jp / oyaizu@waseda.jp

Quinoid polymers have attracted substantial attention as promising organic electrode-active materials due to their fast charge/discharge and high specific capacity based on the multi-electron redox reactions. The electrochemical properties of the quinoid polymers including poly(2-vinylanthraquinone) (PVAQ) and the improvement of the properties by the rational design of the backbones have been reported by our group.[1,2]
Quinoid polymers were newly synthesized and applied as the electrode-active materials of the secondary batteries. The batteries showed reversible charge/discharge reaction, high capacity over 150 mAh/g and good cycle performance which was durable even after 100 cycles. In addition, the fast charge/discharge capability within a few minutes was achieved due to facile charge transport in the electrodes.



References

[1] W. Choi, D. Harada, K. Oyaizu, H. Nishide, J. *Am. Chem. Soc.* **2011**, *133*, 19839-19843.
[2] T. Kawai, S. Nakao, H. Nishide, K. Oyaizu, *Bull. Chem. Soc. Jpn*. **2018**, 91, 721-727.

ABSTRACTS OF POSTER PRESENTATIONS

P 03: The proton trap - a new route to organic energy storage

L. Åkerlund[1], R. Emanuelsson[1], G. Hernández[2], F. Ruipérez[3], N. Casado[3], D. Brandell[2], M. Strømme[1], D. Mecerreyes[3], M. Sjödin[1]
[1]Nanotechnology and Functional Materials, Department of Engineering Sciences, The Ångström Laboratory, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden
[2]Department of Chemistry-Ångström Laboratory, Uppsala University, Box 538, SE-751 21 Uppsala, Sweden
[3]POLYMAT, University of the Basque Country, UPV/EHU, Joxe Maria Korta Center, Avda. Tolosa 72, Donostia-San Sebastian 20018, Spain
lisa.akerlund@angstrom.uu.se

Quinones are interesting compounds concerning high capacity electrical energy storage applications.[1] However, in order to utilize the full capacity of their reduced form, the hydroquinone, needs to be involved. This has been shown problematic in aprotic solvents since the protons diffuse away during oxidation, resulting in an irreversible process. Thus, solving this problem could enable utilization of quinone based materials with higher redox potentials, resulting in higher capacity and a larger variety of possible electrolyte systems. A new way to use hydroquinones for high potential energy storage in organic or metal-organic batteries is by incorporating a proton trap into the material.[2] Additionally, by covalently attaching the side groups to a conducting polymer backbone the solubility and conductivity are no longer an issue, enabling the proton trap to function as cathode material in a battery as visualized in Fig. 1. Also important, as evident from our previous study,[2] is the stability of the linker unit connecting the side groups to the backbone. Here, a new and improved proton trap material is reported.[3] The proton trap system, based on incorporating a proton acceptor into a compound for employing the proton coupled electron transfer in aprotic solvents, enables reversible proton transfer during redox cycling. With this system, the redox processes of hydroquinone compounds can be utilized in many different electrolytes, without relying on coordinating salts (e.g. lithium salts) or protic solvents.

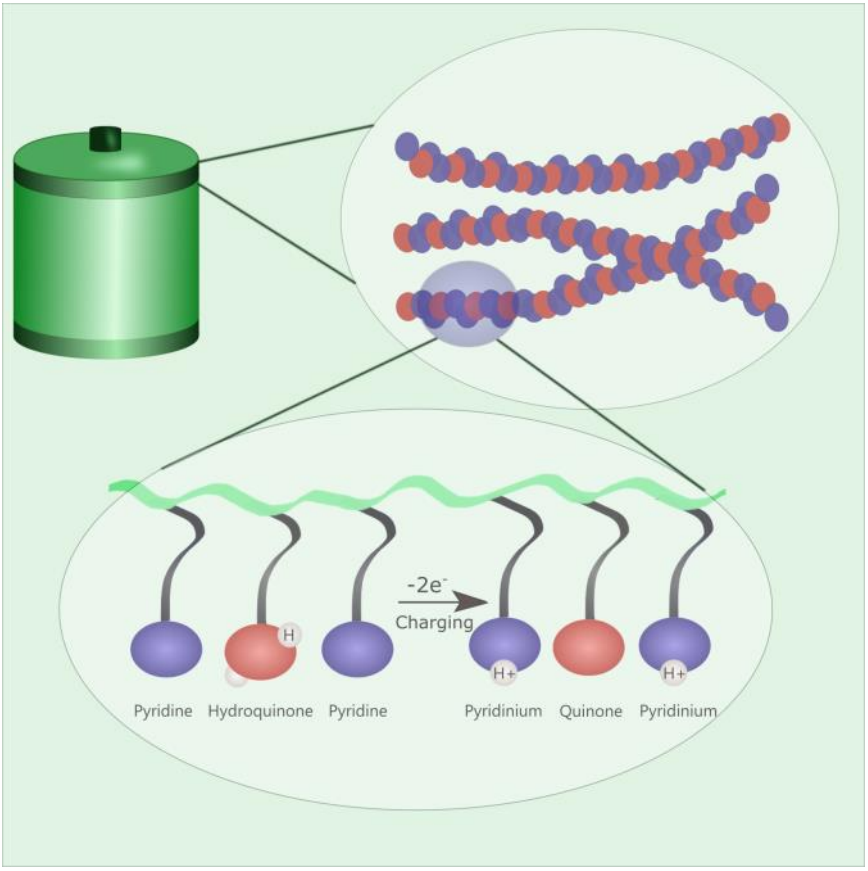


Figure 1. Visualization of a proton trap battery.

References

[1] B. Häupler, A. Wild, U. S. Schubert, *Adv. Energy Mater.* **2015**, *5*, 1402034.
[2] L. Åkerlund, R. Emanuelsson, S. Renault, H. Huang, D. Brandell, M. Strømme, M. Sjödin, *Adv. Energy Mater.* **2017**, *7*, 1700259.
[3] L. Åkerlund, R. Emanuelsson, G. Hernández, F. Ruipérez, N. Casado, M. Strømme, D. Brandell, D. Mecerreyes, M. Sjödin, *submitted*.

ABSTRACTS OF POSTER PRESENTATIONS

P 04: Organic cathode materials for rechargeable Mg batteries

J. Bitenc[1], K. Pirnat[1], T. Bančič[1], A. Vizintin[1], A. Randon-Vitanova[2], R. Dominko[1]
[1]National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia
[2] Honda R&D Europe GmbH, Carl-Legien Strasse 30, 63703 Offenbach, Germany
jan.bitenc@ki.si

Rechargeable Mg batteries are a highly perspective future battery technology. However, development of Mg batteries is connected with two fundamental challenges, first is the incompatibility of Mg metal anode with solvents and salts used in the Li-ion battery electrolytes. Second challenge is the lack of insertion cathode materials. Recent years, have seen quite a significant improvement through the development of several new Mg electrolytes with the improved electrochemical properties (high oxidative stability, non-nucleophilic and non-corrosive), while the progress on the insertion cathode materials remains more elusive.
Organic cathode materials offer a possibility to circumvent issues connected with the difficult intercalation and slow solid state diffusion of Mg cations inside the inorganic hosts. However, their application was until a few years ago limited by the incompatibility between the organic compound, which often contain electrophilic centers, and nucleophilic Mg electrolytes. Our group was one of the first to combine non-nucleophilic Mg electrolytes with organic cathodes, which enabled us to achieve long-term cycling of Mg-organic battery.[1] To investigate the electrochemical mechanism of organic cathodes in Mg batteries we developed a new operando ATR-IR characterization method based on pouch cell with Si wafer window.[2,3] Currently, we are trying to optimize the electrochemical performance of organic cathodes through application of different Mg electrolytes and structurization of cathode materials.

References

[1] J. Bitenc, K. Pirnat, T. Bančič, M. Gaberšček, B. Genorio, A. Randon-Vitanova, R. Dominko, *ChemSusChem* **2015**, *8*, 4128-4132.
[2] A. Vizintin, J. Bitenc, A. K. Lautar, K. Pirnat, J. Grdadolnik, J. Stare, A. Randon -Vitanova, R. Dominko, *Nat. Commun*. **2018**, 9, 661.
[3] T. Bančič, J. Bitenc, K. Pirnat, A. K. Lautar, J. Grdadolnik, A. Randon-Vitanova, R. Dominko, *J. Power Sources* **2018**, *395*, 25–30.

P 05: Isoindoline nitroxide derived high-voltage cathode materials

T. P. Herd, K.-A. Hansen, S. E. Bottle, A. P. O'Mullane, J. P. Blinco
School of Chemistry, Physics and Mechanical Engineering, Science and Engineering Faculty, Queensland University of Technology, Brisbane, Australia
j.blinco@qut.edu.au

Organic radical polymers are a highly promising and environmentally benign class of battery material addressing many of the shortcomings of the more established metal based systems.[1] Herein we report the first examples of polymers based on the isoindoline ring-class as organic electrode materials. Cyclic voltammetry of the nitroxide analogue demonstrated a high oxidation potential of 3.7 V vs. Li, placing it among the highest potential materials in its class. The suitability of the radical polymer for utilisation in a high voltage organic radical battery was confirmed with a large discharge capacity of 104.7 mAh g^{-1} (Figure 1), high-rate performance and stability under cycling conditions (90% capacity retention after 100 cycles).[2] With the fused ring structure allowing easy chemical modification, second generation polymer have been synthesised, making the isoindoline ring-class a very promising candidate for organic p-dopable cathode materials.

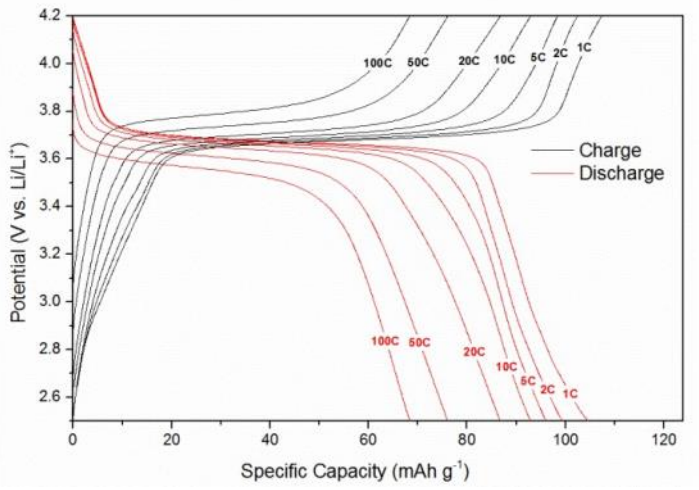


Figure 1. Galvanostatic charge/discharge at different C-rates of lithium-ion coin cell with composite electrode poly(5-vinyl-1,1,3,3-tetramethylisondolin-2-oxyl)/ Super P®/PVDF 10/80/10 wt% in 1 M $LiPF_6$/EC/DEC.

References

[1] K.-A. Hansen, J. P. Blinco, *Polym. Chem.* **2018**, *9*, 1479-1516.
[2] K.-A. Hansen, J. Nerkar, K. Thomas, S. E. Bottle, A. P. O'Mullane, P. C. Talbot, J. P. Blinco *ACS Appl. Mater. Interfaces* **2018**, *10*, 7982-7988.

ABSTRACTS OF POSTER PRESENTATIONS

P 06: Sodium conducting hybrid solid polymer electrolytes for energy storage devices

J. Buchheim[1,2], C. Friebe[2,3], K. Skadell[4], M. Schulz[4], M. Hager[2,3], P. Adelhelm[1,2]
[1]Institute for Technical Chemistry and Environmental Chemistry Jena (ITUC), Germany
[2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Germany
[3]Laboratory of Organic and Macromolecular Chemistry (IOMC), Germany
[4]Fraunhofer IKTS Hermsdorf, Germany
johannes.buchheim@uni-jena.de

The development of rechargeable batteries is regarded as a main key for the overcoming of the so called Energiewende (energy revolution). In view of the respective application, a whole series of requirements must be met like energy density, durability, stability, prize and safeness. Since the launch of lithium ion batteries (LIB) by Sony in 1991 these kind of secondary batteries have be established in the fields of electronic devices, electromobility and stationary energy storage. Organic, aprotic solvents like cyclic and linear carbonates with $LiPF_6$ as conductive salt are used as liquid electrolyte. Even through the advantages of a high ionic conductivity and good electrodes wetting, liquid electrolytes have the main disadvantages of thermodynamically instability towards the normally used electrode materials as well as there inflammability.
In this work we present the preparation and characterization of organic/ inorganic hybrid solid electrolytes for sodium ion batteries (SIB). In addition to the better availability of sodium versus lithium, other advantages like less polarization of interfaces and the prevention of dendrite formation could occur.[1-3] The sodium conducting hybrid polymer consists of polyethylene oxides with different chain length as host for a ceramic filler and a conducting salt. The preparation of the membranes take place by solution casting technique. The characterisation of the solid polymer electrolytes is performed by impedance spectroscopy, X-ray diffraction, differential thermal analysis and cyclovoltametry. The ionic conduction mechanism will be discussed.

References

[1] C. Wadia, P. Albertus, V. Srinivasan, *J. Power Sources* **2011**, *196*, 1593-1598.
[2] P. Adelhelm, P. Hartmann, C. L. Bender, M. Busche, C. Eufinger, J. Janek, *Beilstein J. Nanotech.* **2015**, *6*, 1016-1055.
[3] P. Adelhelm, *Nachrichten aus der Chemie* **2014**, 62, 1163-1168.

P 07: "Water-in-ionic liquids" promoted utilization of redox-active organic materials for flow batteries

R. Chen, Z. Huang, R. Hempelmann
Transfercenter Sustainable Electrochemistry, Saarland University, Germany
ruiyong.chen@uni-saarland.de

Redox flow batteries (RFBs) are regarded as technique-of-choice for load levelling and peak shaving for the utilization of renewable energy sources, and are key component in smart grid networks. With natural abundance, structural diversity and tunability, redox-active organic species as valuable alternatives to the traditional inorganic-based materials are promising to tackle the resource and performance limitations.[1] Conventional RFBs use aqueous H_2SO_4, KOH and NaCl solutions as supporting electrolytes with restricted operating cell voltage and operating temperature. In addition, these typical supporting ions such as Na^+, H^+, SO_4^{2-}, Cl^- and OH^- cannot impose strong interactions with organic solutes.
We have recently developed "water-in-ionic liquid" supporting electrolytes to promote the physiochemical and electrochemical performance of organic materials such as the solubility of active materials and electrochemical reversibility.[2] In our on-going work, we also show that our supporting electrolytes allow a concurrently broadening in the electrochemical and temperature windows.[3] To demonstrate our concept, a class of metal phthalocyanines with electroactive organic ligand rings has been tested as anolyte materials. They show multi-electron transfer reactions at low negative potentials that are not accessible in common aqueous electrolytes. Electrochemical experiments at a broad temperature range from -32 to 65 °C confirm their excellent cyclability.

References

[1] R. Chen, *ChemElectroChem* **2019**, *6*, 603-612.
[2] R. Chen, R. Ye, R. Hempelmann, S. Kim, A. Möller, J. Hartwig, N. Krawczyk, P. Geigle, *Patent application*: PCT/EP2018/056087, **2018**.
[3] Z. Huang, P. Zhang, X. Gao, D. Henkensmeier, S. Passerini, R. Chen, *ACS Appl. Energy Mater.* **2019**, DOI: 10.1021/acsaem.9b00467.

P 08: Natural organic molecular based hierarchically porous carbon for enhanced supercapacitive performance

M. S. Choi, H. S. Park
SungKyunKwan University, South Korea
phs0727@skku.edu

Recently, organic substance based energy technologies are intensively developed due to their beneficial features like abundance, eco-friendly and sustainable. Here is an introduction for a kind of natural organic material, lignin which in a main composition of lignocellulosic structure of lignum and also the second abundant aromatic biopolymer in nature. In this research, the lignin was used as a precursor of electrode material of hierarchically nano-sized porous carbon. Hydrothermal carbonization and chemical activation were engaged to convert precursor to object porous carbon. Since the KOH molecules penetrated deeply through the amorphous organic structure of lignin, a chemical activation reaction was realized which can realize a wide specific surface area. Due to their extremely high specific surface area and hierarchical porous architecture, the result provides exceptional ion and electron transport properties and it is observed to be an advantage for high supercapacitive performance.

ABSTRACTS OF POSTER PRESENTATIONS

P 09: Understanding the structure and electrochemistry of dicarboxylate electrodes from first-principles theory

R. P. de Carvalho[1], C. F. N. Marchiori[1], D. Brandell[2], C. M. Araujo[1]
[1]Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden
[2]Department of Chemistry - Ångström Laboratory, Uppsala University, Box 538, 751 21 Uppsala, Sweden
rodrigo.carvalho@physics.uu.se

The design of high-efficient electrical energy storage (EES) devices is one of the most challenging topics in science and technology of our century. EES have a great impact on how energy is supplied and the way our society consumes it. Hence, we need to move toward environmentally friendly options not only to produce but also to store energy in face of the environmental changes our planet is facing,[1] In this regard, organic materials have drawn significant attention on the past years due to their low-cost, recyclability, possibility to be synthesized from renewable or feedstock as well as their tunable properties.[2] This present work shows a systematic theoretical study, within the density functional theory (DFT) framework of lithiation processes in a set of dicarboxylates, for instance, dilithium acetylenedicarboxylate, dilithium benzenediacrylate, dilithium terephthalate, dilithium thiophenedicarboxylate and dilithium tolanedicarboxylate. In a first step, the molecular approach has been employed to understand the charge transfer, structural changes and thermodynamics upon lithiation reaction. Thereafter, the crystal structures of these materials has been predicted, in both delithiated and lithiated phases, by applying a particularly successful evolutionary algorithm framework interplayed with DFT calculations.[3] In these crystals, there is an organic component acting as a charge reservoir, which is intercalated by a salt layer, showing a preference to stabilize in monoclinic structure. A similar charge reservoir behaviour is obtained in the molecular structure. Moreover, our results indicate that the charge distribution upon lithiation plays an important role in the design of novel organic electrodes.

References

[1] P. T. Brown, K. Caldeira, *Nature* **2017**, *552*, 45-50.
[2] S. E Burkhardt, J. Bois, J. M. Tarascon, R. G Hennig, H. D. Abruña, *Chem. Mater.* **2013**, *25*, 132-141.
[3] C. F. N. Marchiori, D. Brandell, C. M. Araujo, *J. Phys. Chem. C* **2019**, *123*, 4691-4700.

P 10: Phenothiazine and dibenzocyclooctatetraene-based polymers as electrode materials for organic batteries

G. Desmaizieres, B. Esser
Institute for Organic Chemistry and Freiburg Materials Research Center, University of Freiburg, Germany
gauthier.desmaizieres@oc.uni-freiburg.de

As electronic devices, such as cell phones and laptop computers, are becoming more and more powerful, there is a strong demand for new energy storage materials. Lithium-ion batteries, nowadays used in most portable electronics and in electro-mobility, contain toxic metal salts, which have a significant environmental impact.[1]
Organic electrode materials offer many advantages and fulfil the criteria of being non-toxic, mechanically flexible and more sustainable. One major problem in using small organic molecules, however, is their solubility in the electrolyte, which will result in weak cycling performance of the battery. To avoid dissolution one possibility is to incorporate these redox-active molecules into a polymeric structure, which is insoluble in the used electrolyte.[2] Among the manifold redox-active groups, the majority are of p-type and suitable as cathode materials. Phenothiazine-based polymers are interesting cathode materials which exhibit stable cycling behaviors and high working voltages.[3] In order to design high voltage full-organic batteries, it is necessary to develop n-type redox-active materials, which are reduced at low redox potentials. Dibenzocyclooctatetraene-based polymers could be used for this purpose. We herein present redox polymers based on phenothiazine and dibenzocyclooctatetraene for applications in battery systems.

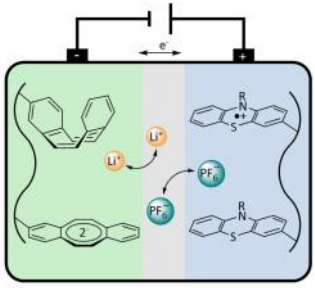


Figure 1: Schematic representation of an all-organic battery containing dibenzocyclooctatetraene- and phenothiazine redox polymers.

References

[1] P. Poizot, F. Dolhem, *Energy Environ. Sci*. **2011**, *4*, 2003-2019.
[2] S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka, U. S. Schubert, *Chem. Rev.* **2016**, *116*, 9438-9484.
[3] M. Kolek, F. Otteny, P. Schmidt, C. Mück-Lichtenfeld, C. Einholz, J. Becking, E. Schleicher, M. Winter, P. Bieker, B. Esser, *Energy Environ. Sci.* **2017**, *10*, 2334-2341.

ABSTRACTS OF POSTER PRESENTATIONS

P 11: Development of high solubility catholytes for organic aqueous redox flow batteries

E. Drazevic[1], C. Szbabo[2], D. Konya[3], A-T. Lindhardt[4], R. H. Nicolaisen[1], T. Lund[5], A. Bentien[1]
[1]Aarhus University, Department of Engineering, Hangoevej 2, 8200 Aarhus N, Denmark
[2]Eotvos Lorand University, Hungary
[3]Research Centre for Natural Sciences, Hungary
[4]Teknologisk Institut, Teknologiparken Kongsvang Allé 29 8000 Aarhus C, Denmark
[5]Department of Science and Environment Chemistry, Universitetsvej 1, 28C.1 4000 Roskilde, Denmark
edrazevic@eng.au.dk

Redox flow batteries (RFB) based on organic redox active species have a low-cost potential for a large-scale electrical energy storage.[1] Several organic molecules seem to be good candidates for the negative side of the RFB, e.g. anthraquinones and viologen derivatives, however, there is no obvious organic candidate for the positive side.[1]

A long-term stable performance of organic RFB was demonstrated with anthraquinone and organometallic species at the positive side, e.g. ferricyanide.[2] Some attempts to utilize organics at the positive side have been reported, e.g. 4,5-dibenzoquinone-1,3-benzene disulfonate, or water-soluble derivatives of 2,2,6,6-tetramethyl-1-piperidinyloxyl.[3] However, these organics are not chemically stable in water. With respect to benzoquinones, this is because fully or partially unsubstituted benzoquinones react with water forming hydroxylated derivatives, which seem to be stable but have a redox potential around 0.4 V.[3] One way to prevent this reaction is to fully substitute the benzoquinone ring. In this work, a new fully substituted hydroquinone was designed and evaluated for the positive side of the organic RFB in symmetric RFB setup. It has four fully protonated morpholino groups, a solubility of 2 M (107 Ah/L) in water and a formal redox potential of around 0.8 V.

References

[1] K. Wedege, E. Dražević, D. Konya, A. Bentien, *Sci. Rep.* **2016,** *6*, 39101.
[2] D. G.Kwabi, K. Lin, Y. Ji, E. F. Kerr, M.-A. Goulet, D. De Porcellinis, D. P.Tabor, D. A.Pollack, A. Aspuru-Guzik, R. G. Gordon, M. J. Aziz, *Joule*, **2018**, *2*, 1894-1906.
[3] L. Hoober-Burkhardt, S. Krishnamoorthy, B. Yang, A. Murali, A. Nirmalchandar, G. K. Surya Prakash, S. R. Narayanan, *J. Electrochem. Soc.* **2017**, *164*, A600-A607.

P 12: Assessing crossover in redox flow batteries: a novel electrochemical method

F. Fenini, A. Khataee, J. Catalano, E. Drazevic, A. Bentien
Department of Engineering, University of Aarhus, Denmark
ffenini@eng.au.dk

Redox flow batteries (RFB) constitute a promising technology for long-duration storage of renewable electricity.[1] Following the recent advances in durability and stability of organic redox couples,[2] all-organic RFB are now regarded as a scalable and cheap technological solution. In this rather stable and simple system, one of the main issues can be the crossover of redox species between the two electrode compartments during operation. The following capacity loss is a major cause of the limited durability of such devices.[3] Here we report a novel experimental procedure with excellent sensitivity to quantify the crossover of redox species during cell operation. The cell is operated filling one of the compartments with milliQ water and then applying squared voltage pulses to reversibly oxidise and reduce the active species in the second compartment. The variation of the total battery capacity as a function of time is used to evaluate the crossover rate. It will be shown how, by varying the period and intensity of the pulse, it is possible to discriminate between migration and diffusion processes originating the crossover of the species. Data will be shown regarding different membranes (Nafion®, Fumasep®) using a model redox couple as ferro/ferricyanide and a potential organic redox couple candidate as AQDS.

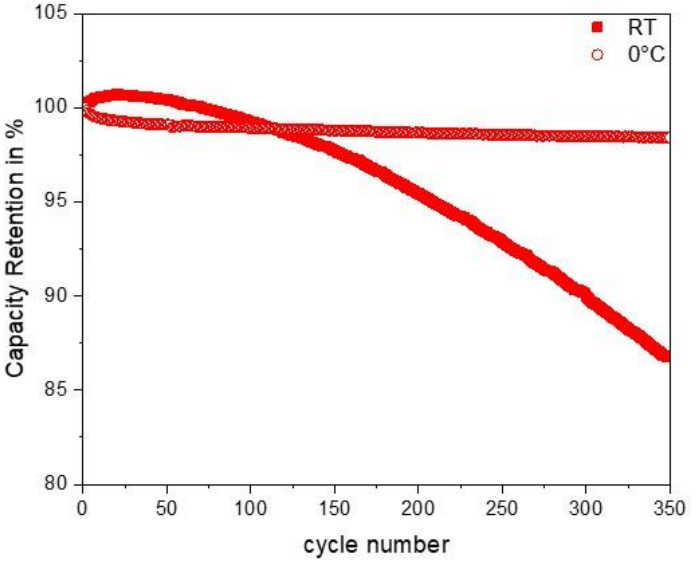
References

[1] A. Khataee, E. Dražević, J. Catalano, A. Bentien, *J. Electrochem. Soc*. **2018**, *165*, A3918-A3924.
[2] D. G. Kwabi, K. X. Lin, Y. L. Ji, E. F. Kerr, M. A. Goulet, D. De Porcellinis, D. P. Tabor, D. A. Pollack, A. Aspuru-Guzik, R. G. Gordon, M. J. Aziz, *Joule* **2018**, *2*, 1894-1906.
[3] R. M. Darling, A. Z. Weber, M. C. Tucker, M. L. Perry, *J. Electrochem. Soc.* **2016**, *163*, A5014-A5022.

P 13: The influence of the salt concentration on the electrochemical performance of electrodes for polymeric batteries

P. Gerlach[1,2], R. Burges[2,3], A. Lex-Balducci[2,3], U. S. Schubert[2,3], A. Balducci[1,2]
[1]Institute for Technical Chemistry and Environmental Chemistry,
Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany
[2]Center for Energy and Environmental Chemistry Jena (CEEC Jena),
Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany
[3]Laboratory of Organic and Macromolecular Chemistry (IOMC),
Friedrich Schiller University Jena, Humboldtstr. 10, 07743 Jena, Germany
patrick.gerlach@uni-jena.de

Redox active polymeric materials, which are cheap, flexible, non-toxic and environmental friendly are good candidates to meet the challenges of modern energy storage applications.[1] Especially organic stable radical polymers (ORPs) have drawn a lot of attention, since they provide fast and simple electron exchange reactions. Thereof poly(2,2,6,6-tetramethylpiperidinyl-*N*-oxymethacrylate) (PTMA), which was first presented by Nakahara et al. in 2002, is one of the most investigated ORPs. It displays a theoretic capacity of 111 mAh/g and proofed high rate capability as well as high cycling stability.[2] In current literature, PTMA is mostly used in combination with the state-of-the-art lithium-ion batteries (LIBs) electrolytes, which are containing a lithium salt dissolved in organic solvents (typically carbonates). However, the actual energy storage process of PTMA has no need for metal-based electrolytes. Therefore, the utilization of PTMA in combination with metal-free electrolytes would be a step towards modern, sustainable, polymeric energy storage systems.
In this work[3] we investigated the performance of PTMA in combination with electrolytes containing different concentrations (1, 2 and 3 M) of the salt 1-butyl-1-methylpyrrolidinium-tetrafluoroborate ($Pyr_{14}BF_4$) dissolved in propylene carbonate (PC) at room temperature and 0 °C. The results of this study indicate that the electrolyte concentration has a strong influence on the capacity, capacity retention and especially self-discharge of PTMA-based electrodes. Furthermore, they also show that the self-discharge performance as well as the cycling stability of PTMA are strongly influenced by the temperature. At 0 °C PTMA-based electrodes are able to display high stability (98% of capacity retention after 350 cycles, see figure) and, at the same, very limited self discharge.

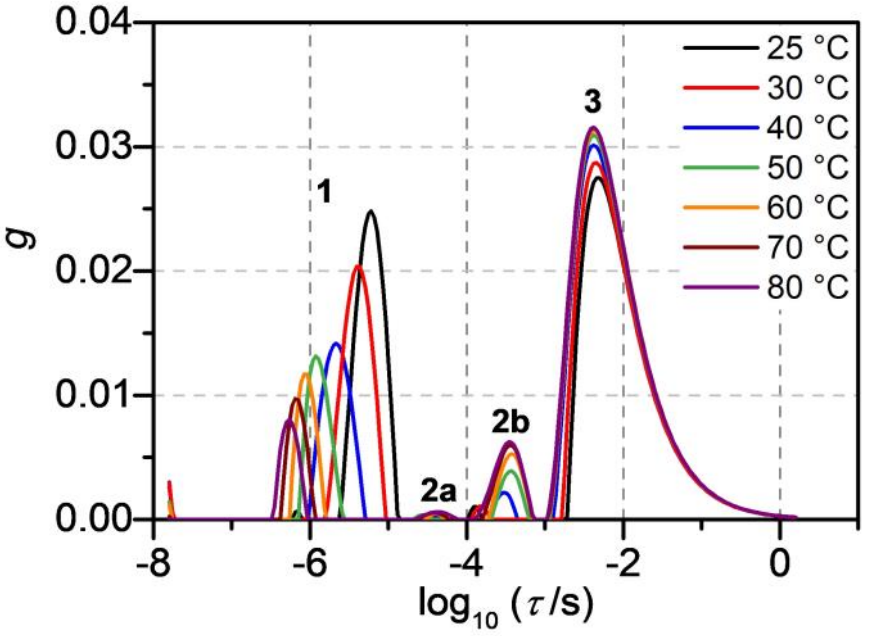


References
[1] C. Friebe, U. S. Schubert, *Topics Curr. Chem.* **2017**, *375*, 19-54.
[2] K. Nakahara, J. Iriyama, S. Iwasa, M. Suguro, M. Satoh, E. J. Cairns, *J. Power Sources* **2007**, *165*, 398-402.
[3] P. Gerlach, R. Burges, A. Lex-Balducci, U. S. Schubert, A. Balducci, *Electrochim. Acta* **2019**, *306*, 610-616.

P 14: Characterizing the ionic conductivity of solid polymer electrolytes using distribution of relaxation times

M. Hahn[1,2], D. Rosenbach[1,3], A. Krimalowski[1,3], M. Thelakkat[1,3], M. A. Danzer[1,2]
University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany
[1]Bayerisches Zentrum für Batterietechnik, Germany
[2]Electrical Energy Systems, Germany
[3]Applied Functional Polymers, Germany
markus.hahn@uni-bayreuth.de

The distribution of relaxation times (DRT) analysis is a model-free, mathematical method offering the possibility to describe the impedance of a resistive-capacitive system by its time constants: A series of n RC elements is used to reconstruct the spectrum obtained by electrochemical impedance spectroscopy measurement.[1,2] The calculation of the resulting distribution function is mathematically ill-posed, however. Thus, regularization is applied using the ec-idea software tool.
In our study, we characterize different polymer electrolytes (SPEs): Brush polymer electrolytes of different nature and degree of polymerization regarding the backbone (m) are investigated, polymethacrylate Poly(MA)$_m$-graft-PEGME$_{1k,2k}$, polynorbornene Poly(Nb)$_m$-graft-PEGME$_{2k}$ as well as different PEG side chain lengths (1k: 1 kg/mol, and 2k: 2 kg/mol).[3] Moreover, single ion-conducting SPEs based on glycidyl propargyl ether (GPE) bearing oligo(ethylene glycol) (OEG), benzyl and LiTFSI side chains are investigated regarding their electrochemical properties. Using coin cells with blocking (steel/copper) and non-blocking (lithium) electrode setups, the ionic conductivity, lithium transport number and the electrochemical stability window is determined. Furthermore, the plating and stripping process within lithium electrodes is visible in the DRT.
The temperature-dependent ionic conductivities are compared and the activation energies are derived from Arrhenius plots. In opposition to e.g. ceramic electrolytes, the DRT reveals that there is only a single conductivity mechanism involved in SPEs so any boundary effects do not contribute to ion transport. This study demonstrates that the DRT analysis is a powerful extension to standard impedance spectroscopy for the identification of conductivity mechanisms and the characterization of transport processes in novel solid polymer electrolytes.



References
[1] M. Hahn, S. Schindler, L-C. Triebs, M. A. Danzer, *Batteries* **2019**, *5*, 43.
[2] A. Weiß, S. Schindler, S. Galbiati, M. A. Danzer, R. Zeis, *Electrochim. Acta* **2017**, *230*, 391-398.
[3] D. Rosenbach, N. Mödl, M. Hahn, J. Petry, M. A. Danzer, M. Thelakkat, *ACS Appl. Energy Mater.* **2019**, DOI: 10.1021/acsaem.9b00211.

ABSTRACTS OF POSTER PRESENTATIONS

P 15: Solar light rechargeable redox-flow batteries

C. Haisch, J. Patzsch, J. Bloh, C. Weidlich
DECHEMA-Forschungsinstitut, Theodor-Heuss-Allee 25, 60486 Frankfurt am Main, Germany
christoph.haisch@dechema.de

Redox flow batteries are widely used to store electricity from photovoltaic cells for later use. Within the joint project "PhotoFlow" the advantages of solar cells and redox flow batteries are combined for the efficient storage of electricity from renewable energy sources in a photo flow battery (Photo-RFB).[1,2] This Photo-RFB directly converts sunlight into stored electrochemical energy by charging the electrolyte at a photoanode. As a starting point, a reference system based on TiO2 as photoanode and aqueous vanadium electrolyte solution has been investigated (Fig. 1). Our aim is to characterise different visible light active photoanode materials and suitable organic electrolytes like TEMPOL (4-hydroxy-2,2,6,6-tetramethylpiperidinyloxyl) to tailor a Photo-RFB system in which photoanode and electrolyte perfectly match each other.[3] Besides the development of a modular cell design, essential information about the limiting factors, cost and efficiency of this new energy storage technology will be collected.

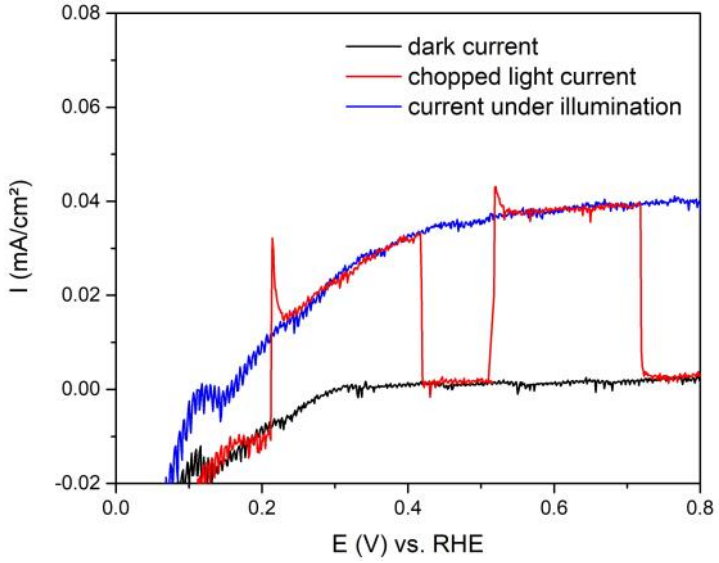


Figure 1: Current-potential curves of a TiO_2 photoelectrode in the "PhotoFlow"-Cell under various irradiation conditions.

"PhotoFlow" is funded by the German Federal Ministry of Economic Affairs and Energy (BMWi) within the government's funding initiative energy storage.

References

[1] J. Azevedo, T. Seipp, J. Burfeind, C. Sousa, A. Bentien, J. P. Araújo, A. Mendes, *Nano Energy* **2016**, *22*, 396-405.
[2] Z. Wei, D. Liu, C. Hsu, F. Liu, *Electrochem. Commun*. **2014**, *45*, 79-82.
[3] B. Huskinson, M. P. Marshak, C. Suh, S. Er, M. R. Gerhardt, C. J. Galvin, X. Chen, A. Aspuru-Guzik, R. Gordon, M. J. Aziz, *Nature* **2014**, *505*, 195-198.

P 16: One-pot synthesis of multidimensional structured 3D nanohybrid material for high performance energy storage

M. Jung, G. S. Gund, H. S. Park
Sungkyunkwan University, South Korea
phs0727@skku.edu

Among the electrochemical energy storage devices, hybrid capacitor has attracted tremendous attention of scientific society due to its amazing feature of high power, good cycle life, tunable energy density, and environmental friendliness. Engineering of active, accessible and safe material with the simple approach is another area of interest in electrochemical energy storage technology. Last two decades, organic materials, especially carbon allotropes like reduced graphene oxide (rGO) and carbon nanotubes (CNTs) have played a great role to enhance performance of energy storage devices due to their special physical and chemical features. Herein, we have attempted one-pot facile synthesis approach to prepare 3D structured nanohybrid material, which have integrated above mentioned key features of electro-active material and thus offered best performance. Our material with new synthesis approach is able to offer optimistic and unmatched ultra-high electrochemical performance.

References

[1] X. Wang, X. Han, M. Lim, N. Singh, C. L. Gan, M. Jan, P. S. Lee, *J. Phys. Chem. C* **2012**, *116*, 12448-12454.
[2] W. F. Zhao, M. Fang, F. R. Wu, H. Wu, L. W. Wang, G. H. Chen, *J. Mater. Chem.* **2010**, *20*, 5817-5819.

P 17: Supercapacitors employing oak-wood-derived porous carbons impregnated with quinones

Y. Katsuyama, Y. Nakayasu, K. Oizumi, Y. Fujihara, H. Kobayashi, I. Honma
Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan
nakayasu@tohoku.ac.jp

With the global warming and depletion of fossil resources, wood-based biorefinery has been attracted. Oak, the most familiar broadleaf tree, used to be felled periodically and utilized sustainably as heat energy resource. However, as the use of fossil fuel increased, the use of wood declined. As a result, more than 40-year-old oak with less CO_2 absorption is easily affected by fungal spores, which is known as a cause of "oak wilt".[1] Once oak wilts, the probability of coppice regeneration decreases.[1] Moreover, the fungal spores chain to nearby healthy oak woods, and forests are rapidly devastated.

In this study, we propose organic redox capacitors composed of wood-bio refined materials for increasing the amount of oak usage. Quinones, which can be synthesized from lignin derived from biomass sources,[2] are used as active materials. Oak-derived activated hard carbons (A-HCs) were used as conductive support materials, fabricated by heat treatment of the hard carbons at 900 °C under CO_2 for 1 hour. Quinones were dissolved in acetone with A-HCs dispersion to adsorb quinones into A-HCs nanopores. Thus obtained composites were mixed with PTFE to serve as electrodes. Electrochemical tests were conducted with 0.5 M H_2SO_4 electrolyte.

A-HCs showed high conductivity (about one order higher than that of conventional activated carbons) and high surface area (1200 m^2g^{-1}). Energy densities of full-cell batteries composed of Tetrachlorohydroquinone (TCHQ) cathode and anthraquinone (AQ) or 1,5-dichloroanthraquinone (DCAQ) anodes were 19.0 Wh/kg and 13.8 Wh/kg, respectively. The utilization rate of AQ was 97.6% (250.9 mAh/g), which was higher than that of our previous works (77%).[3] After 1000 cycles, the discharge capacity was maintained at 91.0% with DCAQ. These devices possessed enough comparable battery performances with previous reports such as lead-acid battery.

References

[1] K. Kuroda, H. Kinuura, K. Osumi, Y. Takahata, *Measures to reduce the damage by oak wilt.*; Japan Forest Research and Management Organization Kansai Affiliate: Kyoto, **2007**

[2] J. C. Wozniak, D. R. Dimmel, E. W. Malcolm, *J. Wood Chem. Technol.* **1989**, *9*, 491-511.

[3] T. Tomai, S. Mitani, D. Komatsu, Y. Kawaguchi, I. Honma, *Sci. Rep.* **2014**, *4*, 3591.

P 18: Exploiting nicotinamide cofactor from natural energy transduction as bio-inspired lithium-ion batteries

J. Kim, S. Ko, C. Noh, H. Kim, S. Lee, D. Kim, H. Park, G.Kwon, G. Son, Y. Jung, D. Lee, C. B. Park, K. Kang
Seoul National University, South Korea
matlgen1@snu.ac.kr

Organic materials are attractive for high energy density, cost effective, and environmentally benign rechargeable batteries. Since organic compounds, especially materials involved in the metabolism of living organisms have long undergone energy conversion and transport processes, they are powerful candidates for energy storage materials.[1]
Herein, we identified the possibility of using the nicotinamide adenine dinucleotide (NAD) motif, which undergoes redox reaction, carrying electrons in mitochondria, for rechargeable lithium ion batteries. Unlike the other reported bio-inspired molecules, the oxidized form of NAD has positive charges. In the case of a biological system, a positive charge of nitrogen can be stabilized by water molecules or other ions in cytosol since molecules are in a dissolved state. However, to be used as a solid organic electrode, it should be stabilized in a different way.
Hence, we used the modified molecule (mNAD), that is formed by removing redox inactive parts of NAD^+ to obtain higher specific capacity and combining with iodide to satisfy the charge neutrality, as a cathode material. In the galvanostatic test, synthesized mNAD-I manifested reversible charge/discharge reaction which showed 2.3 V vs. Li^+/Li of average potential. By comparing the galvanostatic results of some mNAD-X, in addition, which the NAD^+ motif is combined with various halide anions, we demonstrated that the redox reaction of NAD^+ motif was maintained while different species of anions were anchored. Also, we found that the electrochemical properties of mNAD-X electrodes could be tuned by anion characteristics by changing molecular arrangements and electronegativity within electrode. This study implies the potential of utilizing myriad of unexplored bio-derived materials, which facilitate biological energy transductions, as an artificial energy storage system.

References

[1] B. Lee, Y. Ko, G. Kwon, S. Lee, K. Ku, J. Kim, K. Kang, *Joule* **2018**, *2*, 61-75.

P 19: Evaluating organic redox reactants for biodegradable primary batteries for small electronic devices

O. Ibrahim[1], P. Alday[2], N. Sabaté[2,3], J. P. Esquivel[2], E. Kjeang[1]
[1]Fuel cell Research Lab (FCReL), School of Mechatronic Systems Engineering, Simon Fraser University, Canada
[2]Instituto de Microelectrónica de Barcelona, IMB-CNM (CSIC), Campus UAB, Spain
ekjeang@sfu.ca

The continuous rise in electronic devices use is foreseen to cause a significant battery waste generation rate. A new concept of eco-friendly, biodegradable batteries (PowerPAD) for disposable, single-use applications is introduced as a solution that minimizes waste and aligns with circular economy principles.[1, 2] The concept leverages advances in microfluidic cells with flow-through porous electrodes and paper-based membrane-less cells and utilizes organic redox reactants that are internally stored and activated by an aqueous liquid drop and then safely disposed of.
In this work, the reactants requirements are reviewed and a systematic experimental evaluation for their prospective use in PowerPAD is presented, regarding their electrochemical characteristics on carbon electrodes, solubility in aqueous electrolytes, storability in desired redox state and biodegradability. Various half-cell redox couples are ex-situ characterized in various supporting electrolytes using voltammetry techniques to determine their solubility, redox potential and to qualitatively assess their kinetics. A co-laminar flow cell with flow-through porous electrodes is then utilized to in-situ quantify the discharge performance of the selected reactants.
Mixed-media operation, enabled by membrane-less cell designs, is found to allow high voltages and performance output and permit safe disposal by downstream reactants neutralization. Ascorbic acid in potassium hydroxide and parabenzoquinone in oxalic acid are used for the negative and positive half -cells, respectively and yield a maximum power density of 50 mW/cm^2 in-situ. A prototype PowerPAD is finally demonstrated using the same reactants and shows a practical cell voltage >1 V and power of 1.9 mW. The cell performance achieved with biodegradable chemistries provides the departing point for a new class of eco-friendly power sources.

References

[1] J. P. Esquivel, P. Alday, O. A. Ibrahim, B. Fernández, E. Kjeang, N. Sabaté, *Adv. Energy Mater.* **2017**, *7*, 1700275.
[2] O. A. Ibrahim, P. Alday, N. Sabaté, J. P. Esquivel, E. Kjeang, *J. Electrochem. Soc.* **2017**, *164*, A2448-A2456.

P 20: Polyimide/copper hexacyanoferrate - a low cost battery for large-scale energy storage

S. Kjeldgaard[1], L. Najbjerg Skov[1], R. Hestbek Nicolaisen[1], B. Brummerstedt Iversen[2], A. Bentien[2]
[1]Department of Engineering, Aarhus University, Denmark
[2]Department of Chemistry, Aarhus University, Denmark
solveig@eng.au.dk

Increasing the use of sustainable energy sources in the grid presents some challenges in terms of energy storage, due to the highly intermittent nature of sustainable energy sources such as solar and wind power. For batteries to be a viable solution for large-scale energy storage, certain requirements in terms of cost, durability, energy efficiency etc. must be met.
Organic electrode materials are attractive because of their low cost, light weight and electrochemical tunability. Organic redox species can potentially be sourced from biologic material, in contrast to mined inorganics. Since the production could be placed anywhere, it has the further advantage of avoiding geopolitical concerns. Lastly, due to the absence of metals, these materials can simply be disposed of by combustion.
A promising class of organic carbonyl compounds with potential as anode material are polyimides.[1][2] Polyimides are important engineering plastics with high thermal stability and mechanical strength. They are easily synthesized through polycondensation reaction of dianhydrides with diamines. Polymerization lowers the solubility, which is essential as cycling stability requires insoluble electrode materials. Polyimides exhibit a high degree of stability even at high current rates, and can be used in both organic and aqueous electrolyte.
In this work, two types of polyimides are investigated as anode material against a copper hexacyanoferrate cathode with an aqueous Ca(NO3)2 electrolyte.

References

[1] S. Gheytani, Y. Liang, F. Wu, Y. Jing, H. Dong, K. K. Rao, X. Chi, F. Fang, Y. Yao, *Adv. Sci.* **2017**, *4*, 1700465.
[2] P. Sharma, D. Damien, K. Nagarajan, M. M. Shaijumon, M. Hariharan, *J. Phys. Chem. Lett.* **2013**, *4*, 3192 -3197.

P 21: Dissolution/re-deposition processes in poly(vinylphenothiazine)-based li–organic batteries

M. Kolek[1], F. Otteny[2], V. Perner[1], M. Winter[1,3], B. Esser[2,4], P. Bieker[1]
[1]MEET Battery Research Center, Institute of Physical Chemistry, University of Münster, Corrensstraße 46, 48149 Münster, Germany
[2]Institute for Organic Chemistry, University of Freiburg, Albertstraße 21, 79104 Freiburg, Germany
[3]Helmholtz-Institute Münster (HI MS), IEK-12, Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster, Germany
[4]Freiburg Materials Research Center, University of Freiburg, Stefan-Meier-Straße 19, 79104 Freiburg, Germany
martin.kolek@uni-muenster.de

The rising demand for energy storage is facilitating the research on materials for the so-called next generation or beyond lithium ion battery (LIB) technologies. Great potential is assumed for organic-based materials which exhibit low energy densities compared to their inorganic counterparts, but have the ability of fast electron transfer. These high kinetics can lead to increased power densities which could be important for combinations of high energy and high power energy storage in future applications.[1]
Redox polymers are one of the most versatile organic-based materials for energy storage as they show decreased solubility and offer countless possibilities for modifications of the polymeric backbone and the side chains, while the polymer itself can be conjugated or non-conjugated.[1]
Herein, we focus on a non-conjugated redox polymer (PVMPT) with a substituted poly(vinylene) backbone and a methyl phenothiazine moiety as redox active side chain to be used as a cathode material in lithium metal-based batteries. PVMPT undergoes an one-electron transfer process during oxidation while forming a radical cation. The positive charge is balanced by an anion insertion into the polymeric structure.[2]
We performed intensive studies on the working mechanism of PVMPT and could report on a strong π-π-interaction between the side chains which enabled long-term cycling with increased C-rates resulting in an ultra high cycling stability of 10,000 cycles and a capacity retention of 93%.[2]
In this work, we will give further insights into the complex working principle of this polymer. The dissolution of PVMPT will be discussed and a unique re-deposition phenomenon will be presented in detail. Supported by microscopic (SEM, LSM) and spectroscopic experiments (XPS, UV/Vis), the extraordinary cycling behavior of PVMPT is uncovered.[3]

References
[1] S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka, U. S. Schubert, *Chem. Rev.* **2016**, *116*, 9438-9484.
[2] M. Kolek, F. Otteny, P. Schmidt, C. Mück-Lichtenfeld, C. Einholz, J. Becking, E. Schleicher, M. Winter, P. Bieker, B. Esser, *Energ. Environ. Sci.* **2017**, *10*, 2334-2341.
[3] M. Kolek, F. Otteny, J. Becking, M. Winter, B. Esser, P. Bieker, *Chem. Mater.* **2018**, *30*, 6307-6317.

P 22: Bio-inspired molecular redesign of a phenazine-based multi-redox catholyte for high-energy non-aqueous organic redox flow batteries

G. Kwon[1], K. Lee[2], M. Hwan Lee[1], B. Lee[1], S. Lee[1], S.-K. Jung[1], K. Ku[1], J. Kim[1], S. Y. Park[2], J. E. Kwon[2], K. Kang[1]
[1]Department of Materials Science and Engineering, Research Institute of Advanced Materials (RIAM), Seoul National University, 1 Gwanak Road, Seoul 151-742, South Korea
[2]Center for Supramolecular Optoelectronic Materials (CSOM), Department of Materials Science and Engineering, Research Institute of Advanced Materials (RIAM), Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, South Korea
matlgen1@snu.ac.kr

Redox-active organic materials (ROMs) have recently attracted significant attention as potential electro-active components for redox flow batteries (RFBs) to achieve green, safe, and cost-efficient energy storage. In particular, ROMs capable of multi-electron redox reactions at high redox potential have shown great promise for boosting the energy density of RFBs. Further tailoring these ROMs to be highly soluble in non-aqueous media would yield RFB technologies with the highest possible energy density. Herein, we present a highly soluble phenazine-based molecule, 5,10-bis(2-methoxyethyl)-5,10-dihydrophenazine (BMEPZ), that undergoes a reversible multi-electron redox. This molecule was rationally redesigned using inspiration from energy transduction processes in biosystems. The newly designed catholyte material undergoes two single-electron redox reactions at high redox potentials (−0.18 and 0.61 V vs. Ag/Ag^{+}) with remarkable chemical stability and fast kinetics. Moreover, an all-organic flow battery based on BMEPZ exhibits cell voltages of 1.2 and 2.0 V with a capacity retention of 99.94% per cycle over 200 cycles. Notably, the high solubility of BMEPZ results in a flow cell with the highest energy densities (~17 Wh L^{-1}) among non-aqueous all-organic RFBs reported to date.

P 23: Effects of crown ethers on the redox potential of Lithium organic batteries

Y.-F. Yang, C.-Y. Chiou, C.-W. Liu, C.-L. Chen, J.-T. Lee
Department of Chemistry, National Sun Yat-sen University, Kaohsiung 80424, Taiwan
tlee@faculty.nsysu.edu.tw

Tunable electrochemical potential of lithium organic radical batteries without the requirement of structure modification of the redox unit center can be attained with a higher working voltage of the battery through the electrolyte system using various concentrations of the electrolyte salt and the crown ethers. Two different crown ethers were used as electrolyte additives to raise the electrochemical potential of the batteries. The structures and system energies of the Li-crown ether complexes are also investigated by density functional theory (DFT) calculation. Adding one equivalent of crown ether in the Li | PTMA cells can significantly improve the capacity retention up to 21% after 300 cycles at a current rate of 3C.

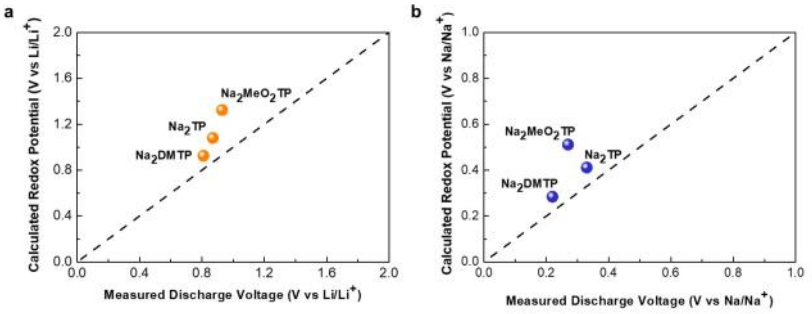
References

[1] K. Nakahara, S. Iwasa, M. Satoh, Y. Morioka, J. Iriyama, M. Suguro, E. Hasegawa, *Chem. Phys. Lett.* **2002**, *359*, 351-354.
[2] H. Nishide; S. Iwasa, Y.-J. Pu, T. Suga, K. Nakahara, M. Satoh, *Electrochim. Acta* **2004**, *50*, 827-831.
[3] H. Tokue, T. Murata, H. Agatsuma, H. Nishide, K. Oyaizu, *Macromolecules* **2017**, *50*, 1950-1958.

P 24: Redox potential dependent on cation-molecular interaction plus electronic effect in organic electrode materials

S. Lee, J. Hong, J. E. Kwon, S. Y. Park, K. Kang
Seoul National University, Department of materials science and engineering, South Korea
matlgen1@snu.ac.kr

Rechargeable batteries based on organic electrode materials are an attractive energy storage alternative in terms of cost-efficiency and sustainability. Feasible chemical modifications of organic materials also offer a tool for their versatile and easily tunable electrochemical properties as electrodes in battery systems.[1,2] Herein, we discuss the effect of substituting functional groups on the redox potential in Li- and Na-ion cells using two novel disodium terephthalate (Na2TP) derivatives. It is shown that the substitution of electron donating functional group generally lowers discharge voltages of organic anode materials by shifting the lowest unoccupied molecular orbital (LUMO) energy, which is consistent with prior knowledge. In contrast, the same substitution is shown to also raise the voltage owing to specific ion interactions with the substituents. The strong binding interaction between the intercalating ion (Li^+) and methoxy substituents significantly lowers the free energy of the discharged products, resulting in elevation of the redox potential despite the high LUMO level of the host molecule. These findings suggest the competition between electronic effects and the ionic interaction as the governing factor determining the redox voltages, providing an important guideline to fine-tune the voltage of new organic electrodes.



References

[1] M. Lee, J. Hong, D. H. Seo, D. H. Nam, K. T. Nam, K. Kang and C. B. Park, *Angew. Chem. Int. Ed.* **2013**, *52*, 8322-8328.
[2] H. Gin, Z. P. Song, H. Zhan, Y. H. Zhou, *J. Power Sources* **2014**, *249*, 367-372

P 25: High-performance radical polymer-grafted graphene composite cathode materials with varying graft density

Y. Li, P. Liu, X. Huang
Shanghai Institute of Organic Chemistry, CAS, China
liyongjun78@sioc.ac.cn

A critical challenge faced by organic radical polymers as cathode materials is how to enhance the electrical conductivity of the cathode with high content of the polymers while to prevent the dissolution of them in electrolyte.[1] Here, we report a facile preparation of radical polymer grafted graphene composite materials, graphene-graft-poly(2,2,6,6-tetramethylpiperidin-1-oxyl-4-yl methacrylate) (RGO-g-PTMA), via the free radical polymerization (FRP) of 2,2,6,6-tetramethyl-piperidin-4-yl methacrylate (TMPM) in the presence of graphene sheets, followed by post-oxidation affording stable nitroxide radicals.[2] The density of grafted polymers was simply tuned by varying the reaction time or the feed ratio of the initiator. Such a structure can inhibit the dissolution of PTMA in electrolyte solution on one hand, and promote electron transport in cathode materials on the other. RGO-g-PTMA based composite cathode with high graft density and a total amount of 10% PTMA shows a reversible specific capacity up to 508 mAh/g at 1C based on the mass of PTMA, which is much higher than the theoretical capacity of PTMA. While the cathode with 15% PTMA and low graft density delivers a high gravimetric capacity of 64.5 mAh/g when normalized to the whole cathode weight. All of the cathodes show good cycling stability and excellent rate performance. The outstanding electrochemical performance, as investigated by galvanostatic intermittent titration technique (GITT) and ex situ electron spin resonance (ESR) spectroscopy, is resulted from the fast two-electron redox reaction of PTMA and the surface Faradaic reaction of RGO, which paving the way for developing high performance organic cathode materials.[3]

References

[1] T. Janoschka, M. D. Hager, U. S. Schubert, *Adv. Mater.* **2012**, *24*, 6397-6409.
[2] L. Kan, Z. Xu, C. Gao, *Macromolecules* **2011**, *44*, 444-452.
[3] Y. J. Li, Z. K. Jian, M. D. Lang, C. M. Zhang, X. Y. Huang, *ACS Appl. Mater. Interfaces* **2016**, *8*, 17352-17359.

P 26: Perylene tetracarboxylic diimide as diffusionless model electrode for organic Na-ion batteries

S. Liebl[1], D. H. Apaydin[2], D. Wielend[3], E. Portenkirchner[1]
[1]Institute of Physical Chemistry, University Innsbruck, Innrain 52c, Innsbruck, 6020, Austria
[2]Linz Institute for Organic Solar Cells/Physical Chemistry, Johannes Kepler University Linz, 4040 Linz, Austria
[3]Institute of Science and Technology Austria (IST Austria), A-3400 Klosterneuburg, Austria
Sebastian.Liebl@student.uibk.ac.at

In this work 3,4,9,10-Perylene tetracarboxylic diimide (PTCDI) is investigated as a cheap, environmental-friendly electrode material for organic Na-ion batteries. The organic material is evaporated on top of a carbon paper substrate with different layer thicknesses ranging from 10-250 nm. The evaporated film is multilayered and consisting of interacting PTCDI molecules. As PTCDI is semiconducting and overall easily accessible for ions to diffuse into the system that is found to behave in a diffusionless mechanism. The measurements indicate that the diffusion of Na ions into the organic film is much faster than the electron transfer from the carbon paper substrate to and throughout the organic film. Hence, the system can be defined as:
(1) Diffusionless: The charge transfer is the current-limiting process.
(2) Multilayered: The charge transfer between the organic molecule layers has to be considered.
(3) Interactive: The system obeys a Frumkin-type isotherm.
Such a system is considered advantageous for investigating kinetic and interactive parameters of the active organic material, as diffusion of the ions into the organic film is not affecting the experimental signals. Laviro[1] theoretically described a multilayer model for space distributed redox modified electrodes, which is similar to the PTCDI-carbonpaper composite electrode system. By evaluating cyclic voltammetry measurements at different scan rates in combination with potential dependent impedance measurements the kinetic and interactive parameters of the PTCDI film can be determined, applying the theoretical insights elaborated by Laviron.
The kinetic and interactive parameters of the PTCDI electrodes obtained in this work are of great significance to other, diffusionless organic electrodes in the field of organic battery research.

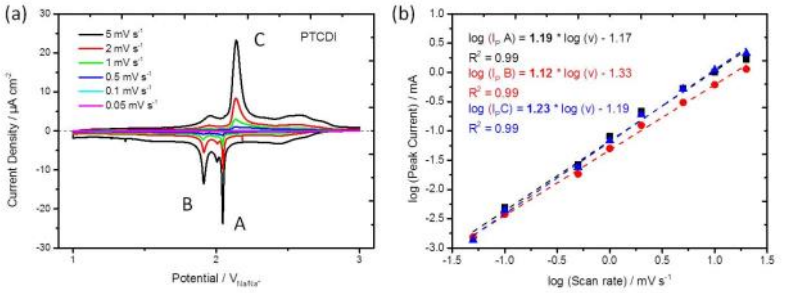


Figure 1: (a) Cyclic voltammogram of PTCDI with various scan rates (5-0.05 mV s^{-1}).
(b) Plot of log(Peak-current) vs. log(Scan rate) with linear fit for the peaks A,B and C.

References

[1] E. Laviron, L. Roullier, C. Degrand, *J. Electroanal. Chem.* **1980**, *112*, 11-23.

P 27: Organic/inorganic hybrid electrode materials: controllable synthesis and battery applications

Y. Lu, J. Chen
Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), Renewable Energy Conversion and Storage Center, College of Chemistry, Nankai University, Tianjin 300071, China
chenabc@nankai.edu.cn

Organic carbonyl compounds have attracted much attention in recent years because of their low cost, high abundance, flexible structural designability, and environmental friendliness. However, pure small organic carbonyl materials are easily dissolved in aprotic electrolyte, leading to inferior cycling stability, low Coulombic efficiency, and undesired shutting problems.[1] We here proposed a series of organic/inorganic hybrid materials and investigated their controllable synthesis and battery applications.[2,3] The organic/inorganic hybrid materials mainly include two types. One is oxocarbon salts which are endowed with high polarity and intermolecular chelate bonds, resulting in limited solubility in aprotic electrolyte. The other is organic/carbon composites whose cycling stability and rate performance could be enhanced effectively because of the strong interactions (physical, chemical, or both) between organic molecules and highly conductive carbon materials. For example, the poly(imide-benzoquinone)/graphene composites synthesized by in situ polymerization showed high reversible capacities of 271 and 193 mAh g^{-1} at 0.1C and 10C, respectively, as well as a high capacity retention of 86% after 300 cycles in lithium-ion batteries. These well-designed organic/inorganic hybrid materials with high electrochemical performance exhibit good prospects for practical battery applications in the future.

References

[1] Y. Lu, Q. Zhang, L. Li, Z. Niu, J. Chen, *Chem* **2018**, *4*, 2786–2813.
[2] Z. Luo, L. Liu, J. Ning, K. Lei, Y. Lu, F. Li, J. Chen, *Angew. Chem. Int. Ed.* **2018**, *57*, 9443–9446.
[3] Y. Lu, Q. Zhao, L. Miao, Z. Tao, Z. Niu, J. Chen, *J. Phys. Chem. C* **2017**, *121*, 14498–14506.

P 28: Macrocycles as organic electrodes materials: a theoretical investigation employing first-principles theory

C. F. N. Marchiori[1], C. M. Araujoa[1]
[1]Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden
c.marchiori@physics.uu.se

Organic electroactive materials (OEM) are promising candidates to be used in the next generation of environmentally friendly battery technologies. Recently, the use of redox-active macrocycles has been proposed as a strategy to overcome these hurdles.[1,2] By controlling the delocalization of the reduced state and minimizing the electron repulsion between adjacent redox active units, Kin and coworkers obtained a well-defined one-plateau voltage profile in a Li-ion battery using a pyromellitic diimide (PMDI) based macrocycle.[1] In another work, the same group reported a very promising application of a phenantrene-quinone-based (PQ) macrocycle in an aluminium battery. They showed that this macrocycle display an improved specific capacity and cyclability as a consequence of the layered structure and minimization of solvent effects.[2] Porphyrins derivatives have also been successfully applied in redox-flow batteries, showing high stability, good conductivity and fast electrochemical kinetics.[3] Motivated by all these studies, we investigate from a theoretical perspective, the electrochemical activity of carboxylate and quinone based macrocycles, including the PMDI and PQ among other such as porphyrins, porphycenes and thiophene-based macrocycles. By comparing the electrochemical properties of this cyclic compounds with their linear analogue we probe the impact of the cyclic conformation on the electronic structure and redox potentials. By using density functional theory calculations (DFT) in a molecular approach, we assess the potential of successive redox processes probing the materials capability of acting as charge reservoir. Additionally, we predict the crystal structure of this materials employing an evolutionary algorithm approach interplayed with DFT calculations, shedding light on how such complexes structures might organize in the solid-state.

References

[1] D. J. Kim, K. R. Hermann, A. Prokofjevs, M. T. Otley, C. Pezzato, M. Owczarek, J. F. Stoddart, *J. Am. Chem. Soc.* **2017**, *139,* 6635-6643.
[2] D. J. Kim, D. J. Yoo, M. T. Otley, A. Prokofjevs, C. Pezzato, M. Owczarek, S. J. Lee, J. W. Choi, J. F. Stoddart, *Nat. Energy* **2019**, *4*, 51-59.
[3] T. Ma, Z. Pan, L. Miao, C. Chen, M. Han, Z. Shang, J. Chen, *Angew. Chem. Int. Ed.* **2018**, *57*, 3158-3162.

P 29: A novel binder-free cathode based on electro-polymerized conductive polymer for Li-S batteries

H. Yu[1,2], S. Mei[1], Y. Lu[1,3]
[1]Institute of Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
[2]School of Advanced Materials, Peking University Shenzhen, China
[3]Institute of Chemistry, University of Potsdam, Germany
yan.lu@helmholtz-berlin.de

Lithium-sulfur (Li-S) batteries hold great potential for next-generation high-performance energy storage systems owing to their high theoretical capacity (1672 mAh g^{-1}), eco-friendliness, and low operation costs as well as the earth abundance of sulfur.[1] Several critical challenges remain with the cathodes of Li-S batteries that limit their commercialization, the most important issue is the rapid capacity fading due to polysulfide dissolution and uncontrolled redeposition. Various nanostructured cathode materials have been reported to improve the electrochemical performances. However, polysulfides still diffuse out for a prolonged time if there is no chemical linking of sulfur species with the host materials. The direct copolymerization of sulfur with highly conductive polymers represents a judicious way to design efficient cathode materials for Li-S batteries.[2] Herein, we explore the synthesis of a functional and conductive polymer poly(4-(thiophen-3-yl) benzenethiol) (PTBE) as sulfur host material to suppress the shuttle effect.[3] The PTBE have been deposited on the surface of Nickel foam by an electropolymerization method, which enables the application of a highly porous and binder-free cathode for Li-S batteries. Sulfur has been copolymerized with PTBE film through inverse vulcanization to form the highly crosslinked copolymer cp(S-PTBE), in which the feed sulfur is chemically bonded to the thiol groups of PTBE. The binder-free cp(S-PTBE)-based cathode exhibits a high discharge capacity and excellent cycling stability, which is ascribed mainly to the conductive pathways of PTBE and the chemical confinement of sulfur through the stable covalent bonds between sulfur and the thiol groups.

References

[1] S. Zeng, L. Li, L. Xie, D. Zhao, N. Wang, S. Chen, *ChemSusChem* **2017**, *10*, 3378-3386.
[2] J. Fanous, M. Wegner, J. Grimminger, Ä. Andresen, M.R. Buchmeiser, *Chem. Mater.* **2011**, *23*, 5024-5028.
[3] B. Boer, H. Meng, D. F. Perepichka, J. Zheng, M. M. Frank, Y. J. Chabal, Z. Bao, *Langmuir* **2003**, *19*, 4272-4284.

P 30: Structure-property relations of quinone-based active materials for redox flow batteries

S. Schwan, J. D. Hofmann, J. Janek, D. Schröder, D. Mollenhauer
Institute of Physical Chemistry, Justus-Liebig University Giessen,
35392 Giessen, Germany
doreen.mollenhauer@phys.chemie.uni-giessen.de

First principles calculations can contribute to the understanding of organic active materials supporting the development of redox flow batteries.[1,2] Quinones have been shown to be especially promising materials for such batteries.[3] Thus, we investigated structure-property relations for different quinone-based molecules by means of DFT calculations. The applied density functional has been benchmarked with a wave function-based method and experimental data to estimate the performance. The effect of the ring size, number and position of substituents and hydrogen bonds have been analyzed in a systematic way regarding the redox potential and stability of the quinone-based active materials. The results of this study provide potential candidates for synthesis and construct design principles of new molecules for redox flow batteries.

References

[1] S. Er, C. Suh, M. P. Marshak, A. Aspuru-Guzik, *Chem. Sci*. **2015**, *6*, 885-893.
[2] J. D. Hofmann, F. Pfanschilling, N. Krawczyk, P. Geigle, L. Hong, S. Schmalisch, H. A. Wegner, D. Mollenhauer, J. Janek, D. Schröder, *Chem. Mater.* **2018**, *30*, 762-774.
[3] B. Huskinson, M. P. Marshak, C. Suh, S. Er, M. R. Gerhardt, C. J. Galvin, X. Chen, A. Aspuru-Guzik, R. G. Gordon, M. J. A. Aziz, *Nature* **2014**, *505*, 195-198.

P 31: Printable gel polymer electrolyte for all-organic batteries

S. Münch, R. Burges, A. Lex-Balducci, U. S. Schubert
Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena
Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstr. 10, 07743 Jena, Germany
simon.muench@uni-jena.de

The possibility to use straightforward and cheap manufacturing techniques like printing or roll-to-roll processing is one of the main advantages of organic batteries and enables customizable and cost-efficient productions in large quantities. However, while research has been focused on novel redox-active electrode materials, other important components, like the electrolyte system were adopted from established technologies, such as lithium or sodium ion batteries.[1] Therefore, electrolytes for organic batteries are mainly based on liquid electrolyte solvents and dissolved salts. However, to take the full advantage of the applicable large-scale manufacturing techniques, not only the electrode materials, but all components, including the electrolyte and the separator, have to be printable as well. In this context, polymer-based electrolytes represent a promising alternative, since they provide sufficient mechanical stability to replace the separator, which further reduces the number of components and costs.
Here, we present a new printable gel polymer electrolyte and its application in an all-organic battery. It consists of several functional monomers for a flexible but mechanically stable polymer matrix, a nano-filler to adjust the viscosity for printing techniques, and an ionic liquid (IL), which provides the ionic conductivity. The formulation can be casted directly on top of an electrode and is subsequently polymerized by UV-polymerization within minutes. Thus, no solvent is necessary, which has to be evaporated after casting. The use of ILs enables a high ionic conductivity at room temperature (in the range of 10^{-4} S cm^{-1}), while the negligible vapor pressure and the high thermal stability are beneficial for the safety.

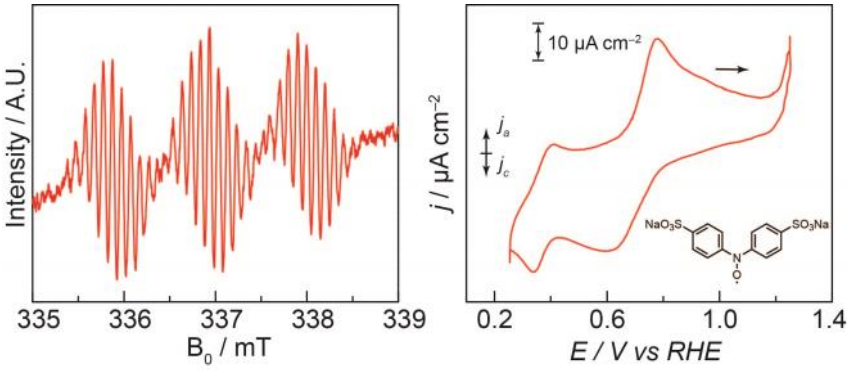
References

S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka, U. S. Schubert, *Chem. Rev.* **2016**, *116*, 9438-9484.

P 32: Electronically tunable redox-active organic mediators

A. T. Murray, H. W. T. Robinson, C. Hoff, N. L. Foss
School of Physical Sciences, University of Kent, United Kingdom
a.t.murray@kent.ac.uk

Redox flow batteries are a highly promising technology for grid-scale energy storage.[1] However, currently most prototypical devices are based on vanadium, which is relatively expensive, possesses poor redox kinetics and is most viable only in highly corrosive, caustic electrolytes. Various proposals have suggested the replacement of vanadium with earth-abundant organic compounds, however many challenges remain including the compatibility of various charged nucleophilic or electrophilic species at various pHs, and crossover i.e. the movement of charge carriers through a supposedly impenetrable membrane leading to irreversible capacity loss.[2] Furthermore, a limited ability to tune electronically redox mediators is a key limitation for some of these species.
Herein we show exploratory approaches to some of these challenges, such as the modification of heterocycles to create `recyclable' mediators, mitigating crossover effects, as well as the use of electronically tunable nitroxyl mediators, allowing alternatives to TEMPO in organic posolyte half-reactions. We also show work towards more unusual energy storage paradigms such as the proposed use of iodine(III) in energy storage and its complex redox chemistry upon variation of proton donor environment.
Overall, this yields a variety of new directions in flow battery technology, as well as other uses of rationally designed mediators such as for catalysis, as spin labels and as fundamental probes of proton-coupled electron transfer.



References

[1] P. Alotto, M. Guarnieri, F. Moro, *Renew. Sust. Energy Rev.* **2014**, *29*, 325-335.
[2] J. Winsberg, T. Hagemann, T. Janoschka, M. D. Hager, U. S. Schubert, *Angew. Chem. Int. Ed*. **2017**, *56*, 686-711.

P 33: Organic secondary battery using neutral aqueous electrolyte solution

Y. Nakagawa, S. Tsujimura
University of Tsukuba, Japan
vfsc72@gmail.com

The development of secondary batteries with high energy density is strongly demanded for wearable electronic devices since the battery size is limited. Unfortunately, inorganic secondary batteries such as lithium ion batteries with high energy density still have a problem in safety for wearable applications.[1,2] Organic batteries gather considerable attentions, but many of them use organic electrolytes, strong acidic or alkaline electrolytes. To solve this problem, we aim to develop an organic battery that operates with a neutral aqueous electrolyte solution. Organic active materials were adsorbed on carbon with high specific surface area. TEMPO derivative was used for the cathodic active material, and anthraquinone and viologen derivatives were used for the anodic active material. These active materials were mixed with Ketjen black EC300, and PVDF in NMP using a tip-type ultrasonicator. The carbon ink was modified on a carbon felt current collector. Phosphate buffer, KCl, NaCl, Na_2SO_4, and $NaNO_3$ was used as model electrolytes (0.25-3 M). Ion exchange membranes and porous membrane were used as a separator. Charge-discharge cycle tests at a constant current (1-20 mA cm^{-2}) were done to evaluate the effect of electrolyte on the performance of the battery. The negative and positive limits of the potential window were −1.8 and 1.8 V vs. Ag|AgCl, respectively, except for KCl and NaCl. The electrochemical oxidation of chloride ion started at 1.3 V. When TEMPO and anthraquinone were used, the cell voltage was 1.5 V. The capacity of the cell clearly depended on the ion characteristics and concentration; the capacity increased as the concentration increased. The sodium nitrate showed the highest capacity among the electrolytes used in this study. The capacity depended not only on the ions passing through the ion exchange membrane but on the counter ions of the electrolyte.

References

[1] Y.-X. Yu *J. Mater. Chem. A* **2014**, *2*, 8910-8917.
[2] M. Miroshnikov, K. P. Divya, G. Babu, A. Meiyazhagan, L. M. Reddy Arava, P. M. Ajayan, G. John, *J. Mater. Chem. A* **2016**, *4*, 12370-12386.

P 34: Aqueous sodium-ion battery with a naphthalene tetracarboxylic diimide (NDI) electrode embedded in a metal-organic framework (MOF)

K. Nakamoto[1], J. Bai[2], L. Zhao[1], R. Sakamoto[2], M. Ito[1], S. Okada[1], E. Yamamoto[3], H. Murayama[3], M. Tokunaga[3]
[1]Institute for Materials Chemistry and Engineering, Kyushu University, Japan
[2]Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Japan
[3]Department of Chemistry, Kyushu University, Japan
s-okada@cm.kyushu-u.ac.jp

Aqueous sodium-ion batteries have gained renewed attention because they can greatly contribute not only to reducing the cost of manufacturing battery but also to development of a broadly distributed energy system. In principle, redox-active molecular organic solids with adequate hydrophobicity may create a suitable electrode/electrolyte interface upon contact with hydrophilic aqueous solution, but such organic electrodes have been less successful in the development of aqueous sodium-ion battery. This is partly because there are virtually not many choices for molecular organic solids showing adequate hydrophobicity over the entire range of their redox state, provided their molecular weight is low. We have recently found a positive effect caused by introducing a MOF structure on the capacity retention in an aqueous sodium-ion battery using a highly concentrated $NaClO_4$ electrolyte and NDI derivatives electrode.
H_2NDI was purchased and used as delivered, while $[Zn(Pyr)_2NDI]_n$-MOF was synthesized from readily available $H_2(Pyr)_2NDI$ and $Zn(NO_3)_2{\cdot}6H_2O$ according to the literature method.[1] Their electrode pellets were prepared by mixing with acetylene black as a conducting carbon and polytetrafluoroethylene binder. Thus fabricated pellets were assembled in three-electrode beaker-type cell with 17 mol/kg $NaClO_4$ aqueous electrolyte. The observed initial capacity of H_2NDI, $H_2(Pyr)_2NDI$ and $[Zn(Pyr)_2NDI]_n$-MOF were roughly equal to their theoretical capacity which was calculated based on $2e^-$ redox reaction (Figure 1a). Although $[Zn(Pyr)_2NDI]_n$-MOF showed relatively smaller capacity since its molecular mass of redox-silent moiety necessarily reduces its theoretical capacity, the capacity retention proved to be excellent, which contrasts sharply with those for H_2NDI or $H_2(Pyr)_2NDI$ with no open framework structure (Figure 1b).

References

[1] C. R. Wade, T. Corrales-Sanchez, T. C. Narayan, M. Dincă, *Energy Environ. Sci.* **2013**, *6*, 2172-2177.

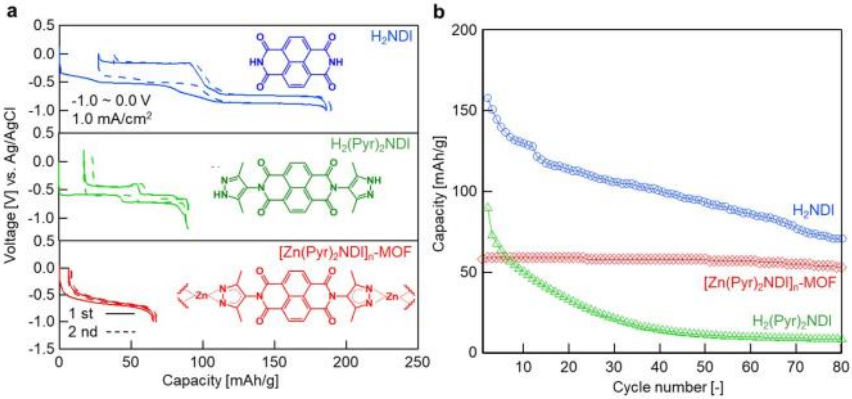


Figure 1. (a) Charge/discharge profiles and (b) cyclabilities of H_2NDI, $H_2(Pyr)_2NDI$, and $[Zn(Pyr)_2NDI]_n$-MOF.

P 35: Eco-friendly cellulose-chitosan hydrogel batteries

M. Navarro Segarra[1], P. Alday[1], N. Sabaté[1,2], J. P. Esquivel[1]
[1]Instituto de Microelectrónica de Barcelona, IMB-CNM (CSIC), Campus UAB, Spain
[2]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Spain
marina.navarro@imb-cnm.csic.es

The proliferation of electrical portable devices has caused an increasing demand of batteries. In particular, the use of primary batteries, such as lithium-ion or alkaline batteries, is producing a dramatic impact in the environment and human health. Despite efforts to implement regulations and social awareness to encourage safe disposal and battery recycling, only 45.7% of the batteries sold in the European Union were collected for recycling during the 2017, with the remaining ones being disposed of in an uncontrolled way.[1] Rethinking the current battery production paradigm becomes mandatory, focusing efforts in finding new biocompatible, biodegradable and environmentally friendly alternatives.[2]

In the past few years, polysaccharides like chitosan, the less acetylated form of chitin, or cellulose derivatives, such as (hydroxypropyl)methyl cellulose, have gained attention for been naturally biodegradable materials. Moreover, these two polysaccharides are the most abundant ones on earth and they have demonstrated extraordinary mechanical and chemical properties, which make them a feasible alternative to petroleum-based polymers.

The work presented herein takes advantage from the water retention capability of these biopolymers to develop a battery. A hydrogel backbone has been synthesized through a solvent casting procedure. This hydrogel matrix allows the gelation of aqueous electrolytes containing different non-toxic redox species and inert salts (such as acetic acid, ascorbic acid, iron nitrate, KCl, KOH) to create the different parts of the battery, i.e. anode, cathode and ion exchange membrane. The components are shaped into a standard coin cell format to obtain a chitosan-cellulose battery. The developed battery meet sustainability principles, using materials that are abundant in nature, requiring small amounts of energy to be produced and being toxic free both during its manufacture and future disposal.

References

[1] Sales and collection of portable batteries and accumulators, Eurostat, March 2019, ISSN 2443-8219
[2] J.P. Esquivel, P. Alday, O.A. Ibrahim, B. Fernández, E. Kjeang, N. Sabaté, *Adv. Energy Mater.* **2017**, *7*, 1700275

P 36: Asymmetric aqueous Li-S capacitor with bisalt soaked poly acrylic acid gel electrolyte and n-doped activated carbon-sulfur(NAC-S)

J. M. Park,[1] M. Jana[1], H. S. Park[1,2]
[1]School of Chemical Engineering, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, South Korea
[2]Department of Health Sciences and Technology, Samsung Advanced Institute for Health Sciences and Technology (SAIHST), Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, South Korea
phs0727@skku.edu

Lithium sulfur battery has become next generation secondary battery, because of its high theoretical capacity(~1675 mAh g^{-1}) and cheap sulfur. However, the organic sulfur battery has some problems; low kinetics, lithium polysulfide shuttling, unsafe and expensive. The unique redox electrochemical behavior of sulfur in aqueous system provides a rational strategy to resolve those problems by designing materials and system.[1] In this research, an unique aqueous sulfur system was tested and applied to a device. Sulfur impregnated N-doped activated carbon (NAC-S) was used as an active material and the electrochemical performance was tested with a three-electrode configuration in aqueous electrolyte. The NAC-S exhibited the capacity around 250 mAh g^{-1} at 4 A g^{-1}. Also, to check feasibility, an asymmetric cell was tested with commercial LMO//bisalt gel//NAC-S system, with bisalt soaked PAAc gel, and showed 26.2 Wh kg^{-1} at 850 W kg^{-1} with 70% retention until the 1000th cycle. Based on this research, the enhanced host material and aqueous system could be implemented in near future.

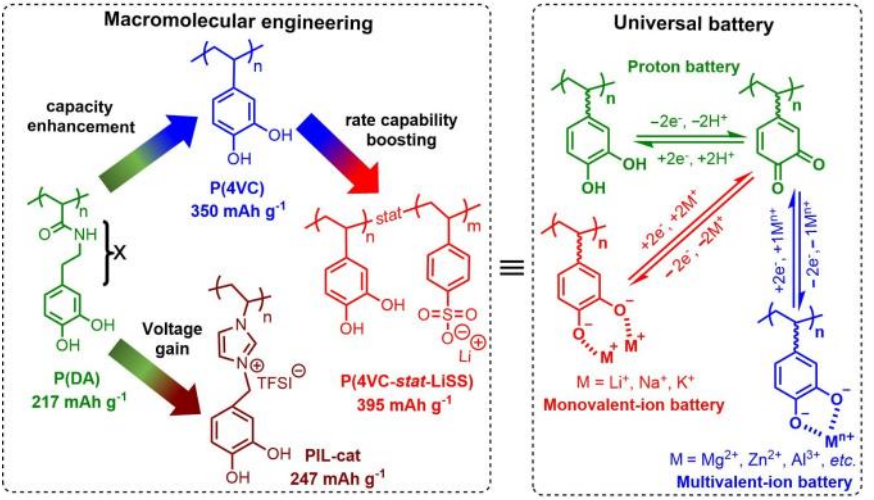
References

[1] C. Yang, L. Suo, O. Borodin, F. Wang, W. Sun, T. Gao, X. Fan, S. Hou, Z. Ma, K. Amine, K. Xu, C. Wang, *Proc. Natl. Acad. Sci. USA* **2017**, *114*, 6197-6202.

P 37: Macromolecular engineering of redox-active polymers bearing catechol pendants: promising paradigm towards high-performance organic batteries

N. Patil, R. Marcilla
Electrochemical Processes Unit, IMDEA Energy Institute, Avda. Ramón de la Sagra 3, 28935 Móstoles, Spain
nagaraj.patil@imdea.org

This decade has been witnessing the resurgence of redox-active polymers (RAPs) in the quest of building large-scale, safe, economical, and sustainable electrochemical energy storage technologies (EESTs) after their brief silence.[1,2] Although numerous RAPs have been successfully applied as electrode materials in EESTs, their macromolecular engineering through controlled/living polymerization methods to design "next-generation" high-performance batteries have been scarcely practiced.
Here, I present the macromolecular engineering of RAPs bearing catechol pendants of different functionality/composition that dictate their electrochemical performances. The classical catechol polymer, poly(dopamine acrylamide) (P(DA)) delivered a specific capacity of 217 mAh g^{-1} in a Li-ion half-cell.[3] Substituting DA repeating units by 4-vinylcatechol (4VC), a smaller structural unit with higher redox-active (RA) atom economy boosted the specific capacity to 350 mAh g^{-1}.[3] Moreover, incorporation of cation conducting styrene sulfonates within the polymer chain in P(4VC-stat-LiSS) drastically improved the rate capability compared to P(4VC).[3] Furthermore, a voltage gain of +350 mV was demonstrated when catechol pendants were confined to an electron-withdrawing poly(ionic liquid) (PIL-cat) backbone, compared to the same RA groups in P(DA).[4] Finally, the universality of catechol-RAPs to reversibly coordinate/uncoordinate numerous cations, ranging from H^+ and Li^+ to Al^{3+} from aqeuous electrolytes will also be discussed.[5] This unprecedented approach is based on a simple catecholato–cation complex (Cat-(mM^{n+}) charge storage mechanism that dictates the overall electrochemistry of the Cat-(mM^{n+})/*ortho*-quinone redox couple: stronger complexes in the order of $M^+ < M^{2+} < M^{3+}$ result in increased redox potentials by hundreds of millivolts.



References

[1] S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka and U. S. Schubert, *Chem. Rev.* **2016**, *116*, 9438-9484.

[2] N. Patil, C. Jérôme and C. Detrembleur, *Prog. Polym. Sci*. **2018**, *82*, 34-91.

[3] N. Patil, A. Aqil, F. Ouhib, S. Admassie, O. Inganäs, C. Jérôme and C. Detrembleur, *Adv. Mater*. **2017**, *29*, 1703373.

[4] N. Patil, M. Aqil, A. Aqil, F. Ouhib, R. Marcilla, A. Minoia, R. Lazzaroni, C. Jérôme and C. Detrembleur, *Chem. Mater*. **2018**, *30*, 5831-5835.

[5] N. Patil, R. Jérôme C. J. Palma, A. Mavrandonakis, C. Detrembleur, R. Marcilla *manuscript submitted.*

P 38: Structural variation of poly(vinylphenothiazine)-based cathode-active materials for rechargeable Li/organic batteries

V. Perner, G. Demaizieres, B. Esser, P. Bieker, M. Winter, M. Kolek
University of Münster, MEET Battery Research Center, Institute of Physical Chemistry, Corrensstr. 46, 48149 Münster, Germany
Institute of Organic Chemistry, University of Freiburg, Albertstrasse 21, 79104 Freiburg, Germany
Helmholtz-Institute Münster, IEK-12, Forschungszentrum Jülich GmbH, Corrensstr. 46, 48149 Münster, Germany
verena.perner@uni-muenster.de

Today the state-of-the-art battery systems are based on lithium ion-based technologies and include transition metal oxides like $LiNi_xMn_yCo_zO_2$ (x+y+z = 1) as active material at the cathode. Despite many advantages, there are some serious drawbacks like the toxicity of the used materials, their lack of sustainability and the high amount of carbon generated during production. Promising candidates for next generation battery systems are organic materials. In comparison to transition metal-based materials, they are prone to be renewable and have a much lower toxicity while less-limited resources are used for synthesis and a lower amount of energy is needed for production.[1]
Despite the drawbacks of a high solubility in common battery electrolytes and low cycle life for organic electrode-active materials, redox polymers have been introduced. These materials contain redox-active units as part of or as side groups at the polymer chain. Most of the reported polymers can be used as cathode-active materials in a so-called “dual-ion” mode. The redox sites should be stable in their oxidation state and decomposition processes should be avoided to reach high cycling stabilities of the battery.[2]
Intensified studies on the redox polymer poly(3-vinyl-N-methylphenothiazine) (PVMPT) were performed which reached an outstanding cycling stability and rate capability. The oxidized redox sites are stabilized via π-π-interactions and a stabilization of the oxidized state of the MPT side chains was identified.[3]
In this work, deeper understanding of the mechanism of charge transport and stabilization of the oxidized state of the polymer will be presented by structural variations of the substituents on the phenothiazine groups. Effects of the polymer structure on the electrochemical behavior as well as on the solubility of the polymer in the electrolyte will be shown.

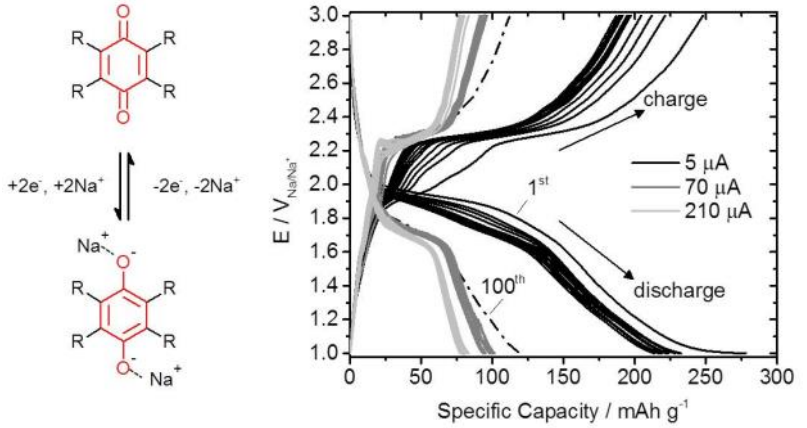
References

[1] Y. Liang, Z. Tao, J. Chen, *Adv. Energy Mater.* **2012**, *2*, 742-769.
[2] N. Casado, G. Hernández, H. Sardon, D. Mecerreyes, *Prog. Polym. Sci.* **2016**, *52*, 107-135.
[3] M. Kolek, F. Otteny, P. Schmidt, C. Mück-Lichtenfeld, C. Einholz, J. Becking, E. Schleicher, M. Winter, P. Bieker and B. Esser, *Energy Environ. Sci.* **2017**, *10*, 2334-2341.

P 39: Quinone based organic composite electrodes for sodium-ion batteries

D. Werner[1], S. Liebl [1], D. Wielend[2], D. H. Apaydin[2,3], E. Portenkirchner[1]
[1]Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria
[2]Linz Institute for Organic Solar Cells (LIOS), Johannes Kepler University Linz, A-4040 Linz, Austria
[3]Institute of Science and Technology Austria (IST Austria), A-3400 Klosterneuburg, Austria
engelbert.portenkirchner@uibk.ac.at

Quinones are a facinating type of battery materials comprising a high theoretical capacity, fast reaction kinetics and a large structural diversity. These excellent qualities are mainly due to their 1,4-benzoquinone units (Fig. 1). Different types of quinones have been considered for nonaqueous and aqueous organic Na-ion batteries.[1] These compounds store charge via an ion-coordination mechanism where the Na-ions coordinate to the negatively charged oxygen atoms upon electrochemical reduction of the carbonyl groups, and uncoordinate reversibly during the reverse oxidation (Fig. 1).
Despite these advantages, mainly dissolution of the active material has hampered their successful application as battery materials. This work presents recent advances using pigments containing benzoquinone units in, for example, anthraquinone (AQ) in comparison to perylene tetracarboxylic diimide (PTCDI) as active material for sodium-ion battery electrodes. Thermally evaporated layers of AQ and PTCDI on a carbon paper substrates are used as electrode composites, whereby the nanostructured carbon adds potential advantages, mainly its large surface area, ordered porous network, large pore volume, good electrical conductivity and low cost.
We demonstrate in this work, that our composite electrodes exhibit reasonable capacity retention and stability in a Na electrolyte system (Fig. 1), attributed to the well-structured intermolecular π-π stacking between the pigment layers and with the subjacent carbon fibers.[2] Their electrochemical characteristics are determined by combining complementary methods, including EIS and CV. FTIR and Raman spectroscopy are employed to probe the composite integrity after galvanostatic charge/discharge cycling.
Similar to inorganic carbon-based materials, like reduced graphene oxide or expanded carbon,[3] quinone-based organic composites may offer a cost-effective, abundant, but also an environmentally benign material for rechargeable Na-ion batteries.



References

[1] B. Häupler, A. Wild, U.S. Schubert, *Adv. Energy Mater*. **2015**, *5*, 1402034.

[2] D. Werner, D.H. Apaydin, E. Portenkirchner, *Battery & Supercaps*. **2018**, *1*, 160 -168.

[3] Y. Wen, K. He, Y. Zhu, F. Han, Y. Xu, I. Matsuda, Y. Ishii, J. Cumings, C. Wang, *Nat. Commun*. **2014**, *5*, 4033.

P 40: Crosslinked polymer electrolytes from imidazolium-based ionic liquid monomers

E.T. Röchow[1], D. Pospiech[1], O. Kobsch[1], M. Coeler[2], K. Nikolowski[2]
[1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden, Germany
[2]Fraunhofer IKTS, Winterbergstr. 28, 01277 Dresden, Germany
pospiech@ipfdd.de

Lithium ion batteries (LIB) are the power source of choice for consumer electronics and are considered the most promising technology for next generation hybrid and electric vehicles. One of the main safety issues in LIB technology arises from using organic compounds such as diethylene carbonate as solvent for lithium salts. Ionic liquids (ILs) are considered alternative, safer electrolytes.[1]

In this contribution, the development of solid state polymer electrolytes is presented, fulfilling the requirements in batteries, i.e. sufficient stability in high-voltage cells and increased safety criteria (non-flammability). In an innovative approach, starting from known imidazolium-based polymeric ionic liquids (PILs), their structure is systematically varied and transformed into mechanically more stable networks. Comparing to poly(vinyl imidazolium) salts, we show two approaches to improve ionic conductivities. First, lowering the glass transition temperature by introducing spacer units, and second, increasing the ion concentration within the monomer structure. Thus, we show monomer and crosslinker syntheses, the subsequent photopolymerization process to obtain self-standing, crosslinked PIL films, as well as the corresponding analytics. In this poster, we show that the synthesized polymer electrolytes are stable up to temperatures >300 °C. The ionic conductivity is significantly increased to 10^{-5} S/cm at room temperature compared to common poly(vinyl imidazolium) structures (10^{-9} S/cm at room temperature). In addition, we also demonstrate the high voltage stability >4.5 V versus Li/Li^+. The concept pursued here can be implemented into organic batteries.

References

[1] B. Scrosati, J. Garche, *J. Power Sources* **2010**, *195*, 2419-2430.

P 41: Reduced graphene oxide /poly(pyrrole-co-thiophene) composite framework for energy storage in supercapacitors

A. A. Shah, S. Ullah
Institute of Chemical Sciences, University of Peshawar, 25120 Peshawar, Pakistan
anwarulhaqalishah@uop.edu.pk

Supercapacitors/ultracapacitors with fast charge and discharge rates are considered as one of the most promising devices for next generation energy storage technologies. This work reports on the preparation of reduced graphene oxide/poly (pyrrole-co-thiophene) (rGO/COP) composites via in-situ oxidative polymerization route for application as active electrode materials in supercapacitor. The composites were analyzed with UV-Vis, FTIR, SEM and XRD for structural, optical and morphological characteristics. The XRD pattern suggested π -π stacking of COP with rGO sheets. The rGO/COP composite showed wrapping morphology with exfoliated rGO sheets acting as the template and COP particles covering the rGO sheets. The specific capacitance of rGO/COP calculated from cyclic voltammetry (CV) curve at 10 mV s^{-1} is 467 F/g while it is 417 F/g calculated from charge discharge curve at a current density of 0.81 A g^{-1}. The capacitance was almost retained up to 200 potential cycling at 10 mV s^{-1}. This study indicates a successful development of rGO/COP composite system to be used as electrode materials for application in supercapacitors.

References

[1] S. Bilal, M. Fahim, I. Firdous, A. A. Shah, *App. Surf. Sci.* **2018**, *435*, 91-101.
[2] S. Bilal, B. Begum, S. Gul, A. A. Shah, *Synth. Met*. **2018**, *235*, 1-15.

P 42: Porphyrinoids as cathode materials for high-performance lithium-ion batteries

S. Shakouri, S. Klyatskaya, M. Ruben
KIT - Karlsruher Institute of Technology, INT - Institute of Nanotechnology, Germany
shirin.shakouri@kit.edu

Porphyrins show an incredibly wide range of magnetic, elctrochemical, photochemical and structural properties. This distinguishes porphyrinoids as a versatile class of molecules. In addition to their application in medicine and solar cell technology, porphyrins are highly suitable as electrode materials. They can be used as cathode or anode material due to their redox behaviour, as we demonstrated recently based on copper-porphyrin [5,15-bis-(ethynyl)-10,20-diphenylporphinato]copper(II) (CuDEPP).[1] They are cheap regarding synthesis and sustainable because the use of rare metals such as cobalt is not necessary.
To gain more understandings of structure-property relationship, we synthesized a series of functionalized porphyrin complexes as electrode material in rechargeable energy storage systems. Based on the CuDEPP,[1] we systematically investigated the influence of different metal centers and meso-substituents.
In this series we examined metal centers such as copper(II), cobalt(II), nickel (II), magnesium(II) and manganese(III) in our porphyrin complexes, and additionally we used boron as a center atom. Along with the influence of copper, cobalt and magnesium as center atoms, we examined the influence of various strong electron-withdrawing groups in meso-position. The electron-withdrawing groups show differences in the inductive and mesomeric effects.
The porphyrins were used as active materials in the cathode, whereas lithium metal was used as the anode material. We were able to see that all compounds are stable during the charge- and discharge processes with a high cyclic stability. Among this, CuDEPP still represents the the highest specific capacity of 210 mAh/g.[1] We found that processability - particularly solubility - plays a crucial role for battery performance.

References

[1] P. Gao, Z. Chen, Z. Zhirong-Karger, J. E. Mueller, C. Jung, S. Klyatskaya, T. Dietmann, O. Fuhr, T. Jacob, J. Behm, M. Ruben, M. Fichtner, *Angew. Chem. Int. Ed*. **2017**, *56*, 10341-10346.

P 43: Binder- and conducting additive-free organic electrode materials - post-deposition polymerization of conducting redox oligomers

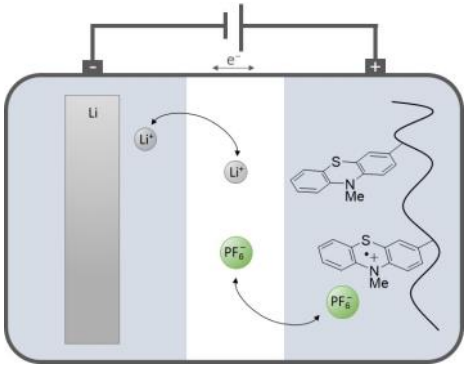
C. Strietzel, M. Sterby, R. Emanuelsson, M. Strømme, M. Sjödin
Nanotechnology and Functional Materials, Department of Engineering Sciences
The Ångström Laboratory, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden
christian.strietzel@angstrom.uu.se

Apart from conventional metal-based batteries, batteries consisting of naturally occurring organic materials can be envisioned, thus becoming fully sustainable and avoiding the negative environmental impact associated with the production and recycling of conventional metal-based batteries. Most organic battery systems being developed today require a substantial amount of carbon- and binder additives, thus often limiting the percentage of active material in the electrode composition to around 50 percent. In this work we show a concept of creating relatively high mass loading of active material, several mg per cm2, on the electrodes without the usage of any additive. Using conducting redox oligomers as starting material, electrodes can easily be coated and polymerization can take place in-situ. While the commercial relevance for this type of material in battery applications still is limited, this system shows interesting properties and constitutes a model for future organic electrode systems. Different types of electrolytes that can be used with this system are discussed.

P 44: Methylphenothiazine-based polymers as Cathode-Active Materials for Organic Batteries

G. Studer, F. Otteny, B. Esser
Institute for Organic Chemistry and Freiburg Materials Research Center, Albert-Ludwigs-University of Freiburg, 79104 Freiburg, Germany
gauthier.studer@oc.uni-freiburg.de

Nowadays, lithium-ion batteries (LIBs) are dominating the electromobility and mobile electronic devices markets. However, these energy storage systems are often based on toxic transition metal oxides, which are produced from scarce natural resources and through energy intensive processes.[1] In view of the growing need of efficient energy storage and in order to achieve a more sustainable society, the development of new battery technologies and electrode-active materials has to be intensified.
Organic compounds are promising candidates for electrode materials in electrochemical energy storage devices, as they can be prepared from renewable resources, are potentially safer and more easily recyclable than classic cathode materials used in conventional LIBs.[2] Nevertheless, many organic materials suffer from dissolution in liquid electrolytes, especially for small organic molecules, leading to capacity decay. To overcome this disadvantage, the solubility can be lowered by attaching the redox-active groups to a polymeric backbone. As previously reported, poly(vinylphenothiazine) exhibited high cycling stability and rate capability at high working voltage.[3] Herein, we present the electrochemical investigations of new redox polymers based on methylphenothiazine, as cathode-active materials for organic batteries.



References

[1] N. Nitta, F. Wu, J. T. Lee, G. Yushin, *Mater. Today* **2015**, *18*, 252-264.
[2] M. Armand, J.-M. Tarascon, *Nature* **2008**, *451*, 652-657.
[3] M. Kolek, F. Otteny, P. Schmidt, C. Mück-Lichtenfeld, C. Einholz, J. Becking, E. Schleicher, M. Winter, P. Bieker, B. Esser, *Energ. Environ. Sci.* **2017**, *10*, 2334-2341.

P 45: Polyimide/multiwalled carbon nanotubes nanocomposite as cathode materials for post Li metal-organic batteries

J. F. Vélez-Santa, T. Bančič, J. Bitenc, R. Dominko
National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia
jf.velez@ki.si

Lithium-ion batteries (LiBs) have proven to be efficient energy storage devices for different portable application. Nevertheless, the ever increasing market demand imposes great requirements such as availability, high energy density, long cycle lives, good safety and low-cost that the current LiBs technologies are unable to satisfy. Post-Lithium-based batteries are called upon to meet these requirement, because they represent a safer, more sustainable and performing alternative to LIBs. Among them, Mg and other abundant metals are attracting the attention of researchers as candidates to replace Li in electrochemical systems due to their abundance, low cost, and high gravimetric and volumetric capacity of their metal anodes. Organic cathode materials are of great interest for application in batteries due to their promising electrochemical performance, high gravimetric capacity and structural flexibility. Such structural versatility enables them to be used as electrodes in different rechargeable batteries including Na, K and Mg. Polyimides (PI) are important engineering polymers with high mechanical strength, excellent thermal stability and those aromatic imides possess reversible electrochemical activity that has already been studied.[1] Here we report on the electrochemical activity of polyimide-based cathodes in different post Li metal-organic batteries. We synthesized two nanocomposites based on 1,4,5,8-Naphthalene-tetracarboxylic dianhydride (NTCDA) and Perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) using ethylenediamine (EDA) as a condensing agent.[2, 3] MWCNT were added during polymerization in order to improve the electric conductivity of these materials and improve the electrochemical accessibility of the electroactive groups within the polymer.[2] Testing in Li electrolytes was used to benchmark the performance of prepared nanocomposites.

References

[1] Z. Song, H. Zhan, Y. Zhou, *Angew. Chem. Int. Ed*. **2010**, *49*, 8444-8448.
[2] T. Gu, M. Zhou, M. Liu, K. Wang, S. Cheng, K. Jiang, *RSC Adv*. **2016**, *6*, 53319-53323.
[3] T. Bančič, J. Bitenc, K. Pirnat, A. Kopač Lautar; J. Grdadolnik, A. Randon Vitanova, R. Dominko, *J. Power Sources* **2018**, *395*, 25-30.

P 46: Investigating an all-organic battery using polyisothianaphthene as a redox-active bipolar electrode material

F.-M. Wang
National Taiwan University of Science and Technology, Taiwan
mccabe@mail.ntust.edu.tw

Polyisothianaphthene has the smallest bandgap among all conjugated polymers and delivers high electrical conductivity. This study uses polyisothianaphthene as an active material to accept both lithium ions and PF_6^- on its cyclic C–S–C bond and benzene ring during the processes of n-doping and p-doping. This study discovers that lithium polysulfide and lithium sulfide are formed during the first electrochemical reaction; however, the impedance, rate performance, and energy density of polyisothianaphthene cells are not affected by those side products. By contrast, an increment of superior rate (10C) testing is significantly improved by those new sulfur-based solid electrolyte interphase formations compared with transitional anode materials, such as graphite, silicon, and other conjugate polymers. The surface characteristics of the polyisothianaphthene electrode are investigated through in situ X-ray absorption spectroscopy, in operando Fourier transform infrared spectroscopy, scanning electron microscopy, and X-ray photoelectron spectroscopy. Furthermore, the reaction mechanisms of n-doping and p-doping on polyisothianaphthene are discussed. The polyisothianaphthene electrode's acceptance of lithium ions exhibits a specific capacity of 730 mAh g^{-1} at the second cycle as well as of 106 mAh g^{-1} when it reacts with PF_6^-. The battery performance exhibits a capacity of approximately 92 mAh g^{-1} when operates in the bipolar mode. The low-bandgap–conjugated polyisothianaphthene is shown to have high reversibility in terms of bipolar electrochemical reactions, which indicates that it can be a promising bipolar organic material for use in lithium ion batteries.

P 47: Side chain quinone redox reaction effects on conductivity of quinone-PEDOT based conducting redox polymer

H. Wang, R. Emanuelsson, M. Strømme, M. Sjödin
Nanotechnology and Functional Materials, Department of Engineering Sciences
The Ångström Laboratory, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden
huan.wang@angstrom.uu.se

Conducting redox polymers (CRPs) have attracted increased interest in recent years due to the possibility of combining the favorable electron transport properties of conducting polymers with the additional functionality provided by the redox active pendent group (PG). Herein we present a series of quinone substituted PEDOT-CRPs where the quinone PGs have been substituted by electron-withdrawing substituents. As expected, introducing electron withdrawing substituents leads to an increase of the quinone formal potential making, for example, CF3-substituted CRPs a promising high-voltage cathode material for lithium ion batteries with a well-defined charge/discharge plateau around 3 V vs. Li^+/Li^0 and 67% retention after 200 cycles. Interestingly, we find a shift in conductivity onset potential concomitant with the quinone formal potential shift indicating that the polymer backbone conductance is intimately associated with the PG redox chemistry. Through in-situ UV-vis, EPR and EQCM experiments as well as by experiments in lithium- and tert-butyl-ammonium based electrolyte we show that the conductance delay is caused by the reduced lithiated quinone state, most likely by localizing the polaron charge carrier as indicated by the EPR experiments.

P 48: Anthraquinone/carbon paper composite electrodes for organic sodium ion batteries

D. Werner[1], D. Wielend[2], D. H. Apaydin[2,3], E. Portenkirchner[1]
[1]Institute of Physical Chemistry, University of Innsbruck A-6020 Innsbruck, Austria
[2]Linz Institute for Organic Solar Cells/Physical Chemistry, Johannes Kepler University Linz, A-4040 Linz, Austria
[3]Institute for Science and Technology Austria (IST Austria), A-3400 Klosterneuburg, Austria
d.werner@student.uibk.ac.at

Sustainability in energy production and storage is becoming increasingly important. Accordingly, in the battery sector, too, there must be a change from rare to natural abundant and ecologically acceptable materials. Since decades scientists attempt to circumvent the lithium's resource problem by searching for alternative active metal ions. A cost-effective and ecologically acceptable alternative to lithium (Li) is the use of sodium (Na) as a carrier ion. Unfortunately, the common electrode materials for Li ion batteries do not work with Na because the inorganic structure of the cathode materials is very sensitive to the larger ion radius of Na. On the other hand the ionic radius has small effects on the electrochemical behaviour of organic material, and carbonyl compounds have been identified as very promising materials for rechargeable ion batteries.[1] In this work we present a water soluble monosubstituted anthraquinone derivative, sulfonated 9,10-anthraquinone (SAQ), as a positive electrode material for Na ion batteries and compare its battery performance with thermally evaporated anthraquinone (AQ) on a carbon paper substrate. SAQ shows a discharge capacity of ~ 95 mAh g^{-1} in the 1st cycle (Figure 1 (a)), while AQ shows a remarkably high discharge capacity of ~ 307 mAh g^{-1}. Both materials were analyzed in different layer thicknesses of active material to study the dependence of the cycle performance on the amount of active material present. SAQ and AQ demonstrate good cycling stability over 100 charge/discharge cycles in a Na-containing electrolyte, wherein the capacity loss of the non-sulfonated quinone is significantly lower compared to the SAQ. One reason for the stable cycling of AQ is expected to result from the stronger π-π stacking interactions of the AQ molecules, which significantly reduces the dissolution of active material into the electrolyte.[2]

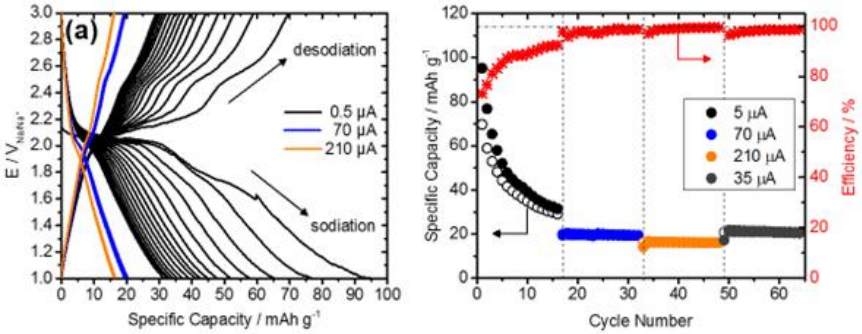


Figure 1: (a) Galvanostatic cycling of SAQ/carbon paper composite with different applied constant currents of 5 µA (black line), 70 µA (blue line) and 210 µA (orange line). (b) Specific capacity and calculated efficiency vs. cycle number at different applied currents of SAQ/carbon paper composite.

References

[1] B. Häupler, A. Wild, U. S. Schubert, *Adv. Energy Mater.* **2015**, *5*, 1402034.
[2] D. Werner, D. H. Apaydin, E. Portenkirchner, *Batteries & Supercaps* **2018**, *1*, 160-168.

.

P 49: Post-polymerization modification for the synthesis of radical containing polymers

W. Xue[1], P. Theato[1,*]
[1]Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology (KIT), Engesser Str. 18, D-76131 Karlsruhe, Germany
* Corresponding authors
patrick.theato@kit.edu

Organic Radical Batteries (ORB) represent an interesting alternative for fast charging batteries. Herein, a post modification method via polymeric active ester was used to fabricate radical containing polymers as a cathode active material in rechargeable batteries. Radical containing polymers with very high radical content of over 90% can be prepared. Additionally, this synthetic route allows for the incorporation of other specific functional groups. Owing to the higher radical content and specific functional groups, problems that hinder the development of radical containing polymers as cathode materials for Li-batteries, such as the lack of suitable synthetic routes that enable a reliable, reproducible and scalable production, self-discharging due to the solubility of radical polymers, poor conductivity can be addressed.

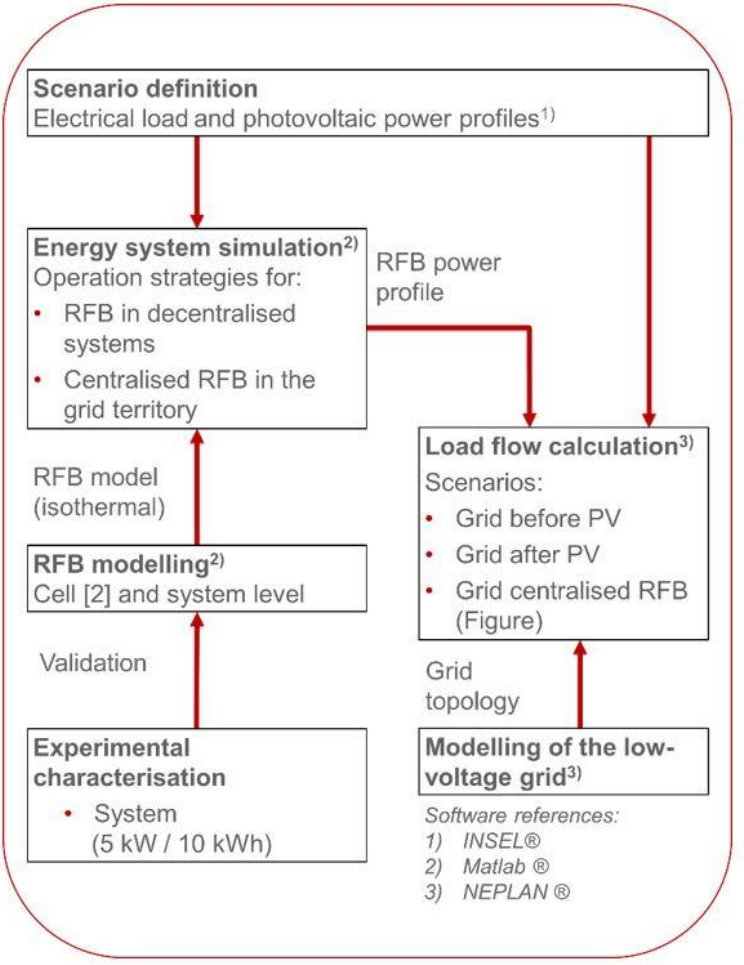
References

[1] S. Muench, A. Wild, C. Friebe, B. Häupler, T. Janoschka, U. S. Schubert, *Chem. Rev*. **2016**, *116*, 9438-948.
[2] H. Nishide, S. Iwasa, Y.J. Pu, T.Suga, K. Nakahara, M. Satoh, *Electrochim. Acta*. **2004**, *50*, 827-831.

P 50: Energy system simulation of redox flow batteries in different applications in the low-voltage grid

C. Zugschwert, S. Dinter, G. Heyer, K.-H. Pettinger, T. Rödiger
Technology Centre Energy, University of Applied Sciences Landshut, Landshut, Germany
Christina.Zugschwert@haw-landshut.de

Historically low-voltage grids (LVG) were built and operated as distribution systems without decentralised energy sources (DES). A high amount of DES due to renewables can cause imbalance between the energy supply and demand. Ultimately LVG operators need to maintain the power quality using control power offered mostly by conventional power plants.[1] The use of energy storage systems (EES) can increase the electrical self-sufficiency of a grid segment and decrease the amount of control power to stabilise the grid. The approach followed here is based on an energy system simulation including a redox flow battery (RFB) model and individual electrical load profiles. The simulations exhibit the RFB power flow within a grid segment and the effects on the grid performance. Therefore, all consumers and sources in the territory need to be defined using individual load and decentralised power profiles. These profiles serve as inputs for the energy system simulation. Within the simulation an RFB model and a control strategy for the battery are combined. The experimental characterisation of a RFB system will provide the data for the RFB modelling and parameterisation. Two different approaches will be investigated within the energy system simulation. The first approach analyses the use of RFBs in decentralised systems and is congruent to the home storage concept for solar energy. The second approach considers only one centralised battery in the territory. Both research approaches offer the potential for different evaluation criteria e.g. load coverage and therefore provide the opportunity to define technical and economic benefits of RFBs in these applications. The output of the simulation are RFB power profiles, which are evaluated in a load flow calculation in order to show the potential of EES to compensate decentralised and fluctuating power suppliers in the LVG.



References

[1] A.-C. Agricola, H. Seidl, S. Mischinger, C. Rehtanz, M. Greve, U. Häger, D. Hilbrich, S. Kippelt, A. Kubis, V. Liebenau, T. Noll, S. Rüberg, T. Schlüter, J. Schwippe, C. Spieker, J. Teuwsen, *dena-Studie Systemdienstleistungen 2030, Sicherheit und Zuverlässigkeit einer Stromversorgung mit hohem Anteil erneuerbarer Energien*. Endbericht, 02/14.

[2] S. König, *Model-based Design and Optimization of Vanadium Redox Flow Batteries*, Dissertation, Karlsruher Institut für Technologie (KIT), **2017**.

made
in
Germany

for more information visit
www.sciospec.com

scio spec

impedance analyzers & potentiostats

flexible. scalable. fully customizable.

from tiny handheld sensor units to large scale industrial test equipment
application specific frontends and sensor interfaces
massive multichannel scalability up to 2048 channels
easily migrate from laboratory to field with fully custom OEM solutions

CONTACT

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

Phone: +49 3641 9-48987
Fax: +49 3641 9-48202
E-Mail: ceec-jena@uni-jena.de

ISBN 978-3-00-062894-8

Publisher: Center for Energy and Environmental Chemistry Jena (CEEC Jena)
Photos: FSU Jena (Jan-Peter Kasper, Anne Günther), pixabay (Stefan Schweihofer), GMK – Medien. Marken. Kommunikation, www.gmk.de
Layout: Communications Office FSU Jena
ISBN 978-3-00-062894-8

www.orgabattdays2019.de