



Annual Meeting of the Danish Electrochemical Society 2023

2nd – 3rd of November





Welcome

We are glad to welcome all the participants to the 2023 Annual Meeting of Danish Electrochemical Society (DEF) held at Technical University of Denmark on 2nd-3rd of November 2023.

We are excited about the reunion as we finally can have a physical annual meeting after the pandemic. We are also excited with the rapid development of electrochemical science and technology in the context of green-transition and growing attention in healthcare during the pandemic. We very much look forward to excellent oral and poster presentations as they are representatives of these recent development.

This year's programme also covers a broad range of aspects of electrochemistry. Moreover, 4 invited oral presentations will be given by: Prof. Alexander Kuhn (Uni. Bordeaux), Dr.-Ing. Steffen Seitz (Physikalisch-Technische Bundesanstalt), Prof. Jonathan Quinson (Aarhus University), and Prof. Søren Højgaard Jensen (Aalborg University).

One of the objectives of the conference is to generate a forum for exchange of knowledge and to strengthen the collaboration between industry and academia. We hope the conference will inspire good discussions and networking between the participants and that all of you will have an interesting and informative conference. DEF is grateful for the sponsorship received from Metrohm Nordic ApS and Elplatek A/S.

Best regards,

The board of the Danish Electrochemical Society:

Paula Sebastian Pascual, chairman
Ming Chen, vice chairman
Sune Veltzé, treasurer
Xinxin Xiao
Anders B Thygesen





Map of the avenue



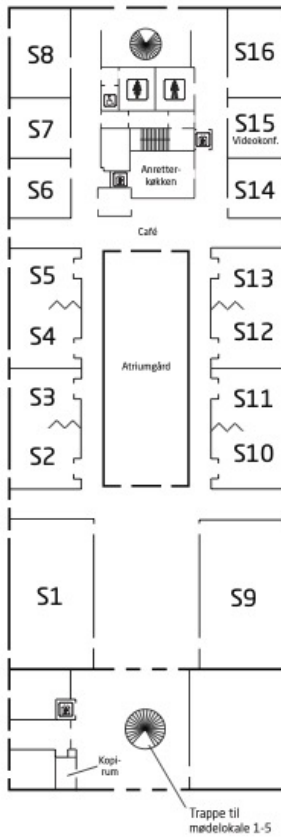
Legend

- Departments
- Oticon Hall
- Administration
- Campus Service
- Halls of Residence and guest houses
- DTU Science Park
- Instructional buildings
- Bus stops
- Canteens
- DTU Library
- DTU Meeting Centre
- DTU Street Food
- ▶ Best access for primary learning facilities





101 (LY101-R3.146MØDERUM_1(111))



Danmarks Tekniske Universitet **DTU**

DTU's Mødecenter

Praktiske oplysninger

Få mere information om DTU's Mødecenter på www.dtu.dk og på Portalen



List of Participants (1/2)

Name	Title	Inst./Co.	E-mail	Abstract
Alexander Kuhn	Prof.	Univ. Bordeaux	kuhn@enscbp.fr	Inv 1
Steffen Seitz	WG-leader	PTB	steffen.seitz@ptb.de	Inv 2
Jonathan Quinson	Asst. Prof.	AU	jquinson@bce.au.dk	Inv 3
Søren Højgaard Jensen	Prof.	AaU	shje@energy.aau.dk	Inv 4
Pradipkumar Leuaa	PostDoc	DTU	pmale@dtu.dk	O 1
Shaofeng Li	PostDoc	DTU	shaoli@dtu.dk	O 2
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Miao Yu	PhD Stud.	DTU	miayu@dtu.dk	P 8

Univ. Bordeaux = University of Bordeaux, PTB = Physikalisch-Technische Bundesanstalt, AU = Aarhus University, AaU = Aalborg University, DTU = Technical University of Denmark, KU = University of Copenhagen, RUC = Roskilde University Center, IRD = IRD Fuel Cells, Metrohm = Metrohm Nordic ApS, Radiometer = Radiometer Medical ApS, Topsoe = Topsoe A/S



List of Participants (2/2)

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Metrohm = Metrohm Nordic ApS, Radiometer = Radiometer Medical ApS, Topsoe = Topsoe A/S



Programme for the 2023 Annual Meeting

Afternoon Thursday, 2nd November 2023

13:00-13:30 Registration

13:30-13:40 Opening

13:40-15:10 1st session

13:40-14:20 Invited talk 1, Alexander Kuhn “Wireless electrochemistry: from materials science to (bio)electroanalysis and beyond”

14:20-14:40 oral 1 Pradipkumar Leuaa “Analysis of overpotentials and ionic transport losses across the zero-gap alkaline electrolysis cells”

14:40-15:00 oral 2 Shaofeng Li “Dynamic interphases for energy storage and conversion”

15:00-15:30 Coffee break

15:30-17:00 2nd session: Battery, Fuel cell

15:30-16:10 Invited talk 2: Steffen Seitz “Using impedance measurements for state of health measurements of second-use Li-ion batteries: Summary of the European metrology research project LiBforSecUse.”

16:10-16:30 Oral 3 Junwei Ding “MOF glass based solid-state polymer electrolyte for lithium metal batteries”

16:30-16:50 Oral 4: Yi-Lin Kao “Polystyrene-b-poly(ethylene-co-butylene)-b-polystyrene (sebs) based bipolar membrane for reverse-bias mode energy conversion system”

17:00-17:45 General assembly of DEF/ Poster presentation

19:00 Dinner at Nørrebro Bryghus



Friday, 3rd November 2023

08:30-09:00 Coffee & breakfast

09:00-09:10 Opening of the 2nd day

09:10-12:10 3rd session: Electrocatalysis

09:10-09:50 Invited talk 3: Jonathan Quinson “Surfactant free (precious metal) nanoparticles: challenges and opportunities for electrocatalysis”

09:50-10:10 Oral 5: Yang Hu “In-operando investigation of catalysts for oxygen electrocatalysis”

10:10-10:30 Oral 6: Heine Anton Hansen “Atomic scale simulations of reactions at gold-water interfaces”

10:30-10:50 Oral 7: Xianbiao Fu “electrochemical nitrogen activation for ammonia synthesis”

10:50-11:10 Coffee break

11:10-11:30 Oral 8: Benedikt Axel Brandes “Rationalizing the electrochemistry of multistep reactions in general and the HOR/HER on platinum in particular”

11:30-11:50 Oral 9: Sarmad Iqbal “Exploring the activity-stability landscape of Ni_{1-x}Fe_x-LDH (x = 0-0.33) for the oxygen evolution reaction at industrially relevant alkaline electrolysis conditions”

11:50-12:10 Oral 10: Thu P. A. Phan “Mechanical alloying of nickel-based catalysts for alkaline water electrolysis”

12:10-13:30 Poster presentation and lunch

13:30- 4th Session: SOEC

13:30-14:10 Invited 4: Søren Højgaard Jensen “Electrothermal balanced operation - A new operation method for improved SOEC performance”

14:10-14:30 Oral 11: Daniel B. Drasbæk “Identification and quantification of degradation in commercial solid oxide electrolysis stacks using the power of electrochemical impedance spectroscopy”

14:30-14:50 Oral 12: Yun Xie “Zinc triggers favorable hydrogenation reactions of air electrodes in protonic ceramic cell”

14:50-15:10 Closing remarks and award ceremony



Short biographies and abstracts – Invited speakers



Short biography – Alexander Kuhn



Alexander Kuhn, University of Bordeaux, France

Alexander Kuhn obtained his diploma degree in chemistry, after studying in Munich, Bordeaux and Oxford, from the Technical University Munich (1991), and his PhD from the University of Bordeaux, (1994). After his post-doc with Fred Anson at the California Institute of Technology (1996), he was appointed in the same year as an Assistant Professor at the University of Bordeaux and then in 2000 as a Full Professor, working now at the Institut of Molecular Science (University Bordeaux, CNRS, Bordeaux INP). Since 2015 he is also Adjunct Professor at VISTEC, Thailand, and more recently (2020) Distinguished Professor of the “Outstanding Talent Program” at Henan University, China. He is a senior member of the Institut Universitaire de France, distinguished senior member of the French Chemical Society and Fellow of the International Society of Electrochemistry. He has been or is still member of the international advisory boards of several journals, *Anal. & Bioanal. Chem.* (2007-2010), *Bioelectrochemistry* (2007-), *Electroanalysis* (2012-), *Electrochim. Acta* (2013-2017), *ChemPhysChem* (2015-), *Sci.Rep.* (2015-), *ChemElectroChem* (2018-), *Microchim.Acta* (2020-), and was also Chair of the editorial advisory board of *ChemPhysChem* (2019-2022). He has served, among others, as council member of the european division of the Electrochemical Society (2006-2008), council member of the electrochemistry division of the French Chemical Society (2016-2018), chair of the bioelectrochemistry division of the International Society of Electrochemistry (2011-2012) and as council member and treasurer of the Bioelectrochemical Society (2008-2019). He is the recipient of several honors, including a fellowship from the Alexander-von-Humboldt foundation, the electrochemistry award of the French Chemical Society and the national science medal in silver of CNRS. His current main research interests are modified electrodes with a special focus on applications in electroanalysis, bioelectrochemistry and electrocatalysis; bipolar electrochemistry; nanomaterials; micromotors; Janus particles; chirality.



Invited 1

WIRELESS ELECTROCHEMISTRY: from materials science to (bio)electroanalysis and beyond

Alexander KUHN¹

¹ Univ. Bordeaux, CNRS, Bordeaux INP, F 33607 Pessac, France
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Wireless electrochemistry, more scientifically also called bipolar electrochemistry, is a concept based on the fact that two opposite chemical processes, oxidation and reduction, occur simultaneously on the surface of a (semi)conducting object, without connection to a power supply [1]. We distinguish between exogenous bipolar systems, for which the primary driving force originates from an external electric field, and endogenous bipolar objects, where an asymmetric chemical composition provides the necessary thermodynamic power to induce spatially separated reactions. The basic phenomena have already been described and used for a long time, but regained interest in recent years, because it became apparent that bipolar electrochemistry has attractive features for developing new applications in various areas. This is mostly due to several advantages over classic electrochemistry, such as the absence of an ohmic contact, the generation of a dual gradient of electroactivity on the same object and the possibility to address simultaneously thousands of objects. Also, some features of this type of electrochemistry allow performing experiments which simply cannot be done with a classic electrochemical set-up.

The objective of this presentation is to introduce first the basic aspects of bipolar electrochemistry, and then to illustrate some recent applications of this concept studied in our group, ranging from materials science^[2-4] and (bio)electroanalysis^[5-8], to the generation of motion^[9-14] and electrosynthesis^[15,16].

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- [8] S. Arnaboldi, G. Salinas, A. Karajic, P. Garrigue, T. Benincori, G. Bonetti, R. Cirilli, S. Bichon, S. Gounel, N. Mano, A. Kuhn, **Nat. Chem.** 13 (2021) 1241
- [9] B. Gupta, L. Zhang, A.A. Melvin, B. Goudeau, L. Bouffier, A. Kuhn, **Chem. Sci.** 12 (2021) 2071
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Short biography – Steffen Seitz



Steffen Seitz, Physikalisch-Technische Bundesanstalt (PTB), Germany

I have a degree in physics and a PhD in electrotechnical engineering. I have been working in the field of metrology in electrochemistry at PTB since 2007, becoming head of the electrochemical working group at PTB in 2015. I am mainly occupied with the optimization of existing and the development of new primary methods for electrochemical measurement quantities, like pH, electrolytic conductivity, ion activity and impedance spectroscopy. Currently, the research focus of my working group is on the pH of seawater in the context of climate change, and on the characterisation of Li-ion battery states by electrochemical impedance spectroscopy. I have participated in several European metrology research projects. The project 'LiBforSecUse' I am going to talk about at the Annual meeting for the Danish Electrochemical Society has been coordinated by me. Furthermore, I am representing PTB in national and international institutions with respect to electrochemical measurands. Since 2019, I am chair of the Working Group for Electrochemical Analysis and Classical Chemical Methods at the International Bureau for Weights and Measures (BIPM).



Invited 2

Using impedance measurements for state of health measurements of second-use Li-ion batteries: Summary of the European metrology research project LiBforSecUse.

Dr.-Ing Steffen Seitz¹

¹Physikalisch-Technische Bundesanstalt (PTB), Germany, Steffen.Seitz@ptb.de

An overview on the main activities and outcomes of the European metrology research project “Quality assessment of electric vehicle Li ion batteries for second use applications” (LiBforSecUse) will be presented. Impedance-results of life-cycle tests of a number of commercial Li-ion battery cells, measured under reproducibility conditions, have been investigated with different kinds of impedance-based evaluation methods. Aging parameters have been identified based on a statistical correlation model that has been adapted for this purpose. The impedance-based evaluation methods have finally been used to develop four empirical models to predict the residual capacity, i.e. direct impedance evaluation, equivalent circuit fitting, analysis of distributed relaxation times and analysis of non-linear frequency response. Each of the models has pros and cons with respect to its application. However, they have proven to be consistent and have shown equivalent ability to predict the residual capacity. A statistical assessment of the predicted residual capacity has shown a mean deviation smaller than 1.5 % from the actual capacity, if the models are applied to the impedance-data used for model development. The robustness of the models has been validated with the data from additional life cycle tests measured with varying cycling conditions, revealing an increase of the deviation up to 5 %. After optimising the models, the mean deviation was smaller than 3 %.

The above-mentioned activities have been supported by the development of low-impedance standards ($m\Omega$ range) to improve the quality of the impedance measurements, by post-mortem analysis to get deeper insight into the aging mechanism of the investigated cells and by physicochemical simulation models to substantiate the empirical models.

The focus of the presentation will be set on the impedance-based measurements and evaluation models for state health prediction. The supporting activities will be summarised to some extent.



Short biography – Jonathan Quinson



Jonathan Quinson, Aarhus University, Denmark

I studied at ESPCI (MSc), Paris, FR, and Imperial College London (MRes), UK, before completing a PhD at the University of Oxford, UK. I then joined the University of Copenhagen (DK) for several postdocs in different groups, in particular under a Marie Skłodowska-Curie Individual Fellowship. Under a Marie Skłodowska-Curie Global Fellowship I stayed 6 months at the University of Stanford, USA. I am now a Tenure Track Assistant Professor at the Biological and Chemical Engineering Department, Aarhus University, DK, leading the Nanomaterials Engineering for Sustainable Technologies group (NEST).

The common theme in my research activities is the development of nano-materials as (electro)catalyst or catalysts supports. In particular, I focused over the years on surfactant-free colloidal syntheses for their relevance to both fundamental and applied research.



Invited 3

SURFACTANT FREE (PRECIOUS METAL) NANOPARTICLES: CHALLENGES AND OPPORTUNITIES FOR ELECTROCATALYSIS

Jonathan QUINSON

Biological and Chemical Engineering Department, Aarhus University, Denmark

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In this presentation, I will try to convince you that “surfactant-free” colloidal syntheses of nanoparticles (NPs) bear promising and maybe under-exploited features for (electro)catalysis [1].

I will start by providing an overview of the different approaches to obtain “surfactant-free colloidal” NPs, with an emphasis on precious metal NPs [1]. I will then stress the relevance of these materials to explore the design of nano-catalysts “beyond the active site”, i.e. including the synthesis of the materials, their processing, and their evaluation, in a holistic approach [2].

The talk will focus on recent achievements made possible by using a polyol-based synthesis for the design of supported platinum (Pt) NPs for the oxygen reduction reaction (ORR) [3]. The advantages of using mono-alcohols over polyols for the synthesis of surfactant-free colloidal NPs will be stressed, e.g. with the example of iridium (Ir) NPs for the oxygen evolution reaction (OER) [4]. Finally, the opportunities stemming from the synthesis of gold (Au) NPs in low boiling point solvents will be introduced, e.g. for alcohol-electro-oxidation reactions [5,6].

I will finally open on the remaining challenges related to the synthesis and use of surfactant-free colloidal syntheses of precious metals NPs, for both fundamental and applied research.

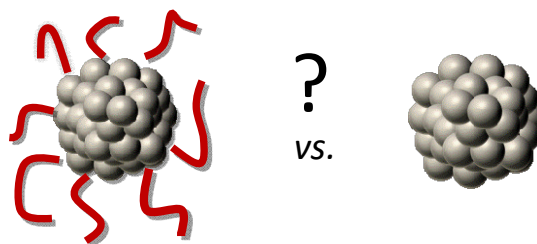


Figure 1. The question of surfactant-free nanoparticles for electrocatalysis.

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Short biography – Søren Højgaard Jensen



Søren Højgaard Jensen

Chief Technical Officer
Founder
Advisor
Professor



AALBORG UNIVERSITY
DENMARK

Profile

Dr. Søren Højgaard Jensen is a globally recognized expert in the field of high-temperature electrolysis for Power-to-X. Power-to-X uses electricity from renewable energy sources to convert water into valuable CO₂-neutral green fuels.

Since 2001, Dr. Jensen has led research and development projects focusing on pressurized operations with high-temperature solid-oxide electrolysis (SOE). He has led and coordinated multiple research projects addressing manufacturing, upscaling, and testing of SOE systems (including cells and stacks).

Additionally, Dr. Jensen consults and lectures within electrochemistry, specifically on solid-oxide cells, batteries, and impedance spectroscopy. He is sought after to supervise the MSc, PhD and post-Doctorate students regarding degradation mechanisms, energy conversion, and energy storage.

Most recently, he has developed and patented a ground-breaking method to operate SOE-based Power-to-X systems. This discovery inspired Prof. Jensen to found Dynelectro which he owns and operates with a high-performance team.

Education

Technical University of Denmark	Early Impact, Accelerator Program (selective), cohort 2021
Ph.D, Physics	Technical University of Denmark, Solid Oxide Electrolyser Cell, 2006
M.Sc., Physics & Mathematics	University of Copenhagen, 2003

Professional

Chief Executive Officer	Dynelectro	current
Chief Technical Officer	Dynelectro, Power-to-X (technology startup), Denmark	current
Board Executive	Dynelectro	current
Professor MSO (20%)	Aalborg University, Department of Energy Technology	2019-current
Advisor	Danish Technological Institute, Energy Storage & Conversion	2019-current
Scholar, Visiting	Colorado School of Mines, Mechanical Engineering	2019-20
Chairman	Danish Battery Society	2013-16
Scholar, Visiting	Northwestern University, McCormick School of Engineering	2012-13
Scientist, Sr.	Technical University of Denmark, Energy Conversion and Storage	2011-18

Achievements

Patents: 4; Peer-reviewed articles: 67; H-index: 27; Citations: 4,521 ([Scopus.com](https://scopus.com); 10-Oct-23)



Invited 4

Electrothermal balanced operation - A new operation method for improved SOEC performance

Søren Højgaard Jensen^{1,2,*}, Thomas Lyck Smitshuysen², Martin Nørby Nielsen², Jan Pieter Ouweltjes³, Dario Montinario³, Mogens Mogensen⁴

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²*DynElectro ApS, Denmark*

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The ongoing green energy transition increases the need for dynamic and efficient Power-to-X (PtX) systems to convert surplus wind and solar power to high-value products. The solid oxide electrolysis (SOE) technology offers the highest energy conversion efficiency. However, operation at part-load, *i.e.* below thermo-neutral potential, creates thermal variations causing thermomechanical stress. Combined with limited lifetime this impedes commercialization of the technology. Here we present a novel operating method that alleviates temperature variations in the SOECs and decreases degradation.

A flat thermal profile across SOE stacks is obtained by switching several times per second between electrolysis mode and brief pulses in fuel cell mode; the thermal mass of the SOE stack prevents temperature fluctuations during the short switching period. The operation method is referred to as AC:DC operation.

In this presentation we present experimental results from an ongoing +1year test of a commercially available G8-80 stack from SolydEra stack with a nominal power of 4.5 kW in electrolysis mode. The observed reduction in the degradation rate is believed to be caused by desorption of impurities that otherwise absorb and agglomerate on the active three phase boundaries of the electrodes. Finally, we discuss how AC:DC operation can enable dynamic operation of large SOE systems.



Abstracts – Oral presentations



ANALYSIS OF OVERPOTENTIALS AND IONIC TRANSPORT LOSSES ACROSS THE ZERO-GAP ALKALINE ELECTROLYSIS CELLS

**Pradipkumar Leuaa¹, Mikkel Rykær Kraglund¹ and Christodoulos
Chatzichristodoulou¹**

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Alkaline electrolysis (AE) is one of the most promising technologies for large-scale green hydrogen production. Although AE has been advanced over the last decade, the costs of hydrogen produced from AE is still very high and economically less competitive compared to other hydrogen production technologies such as methane steam reforming. The current design of AE cells also plays a role in poor efficiency. To design a more efficient AE cell, it is necessary to identify the source of voltage losses across the full cell. Moreover, porous electrode theory considerations suggest that mass transport plays an important role in terms of influencing electrode performance. Therefore, to design more efficient and productive AE cells, identification of electrode architectures which facilitate mass transport and thereby reduce associated ionic transport losses in the electrodes are essential. Here we propose a method that employs a minimum of three reference electrodes (RE) to separate the voltage losses within the anode, cathode, and separator during zero-gap operation at industrially relevant conditions, as well as to deconvolute the Galvani potential losses ($\Delta\phi$) associated with ionic migration within each of the electrodes and the separator. Different Ni electrode structures have been investigated to assess the effect of thickness, surface area, and porosity. Overall, the proposed methodology can guide the rational design of improved electrode microstructures and lead the way to the development of more efficient and productive alkaline electrolysis cells in the future.



Dynamic interphases for energy storage and conversion

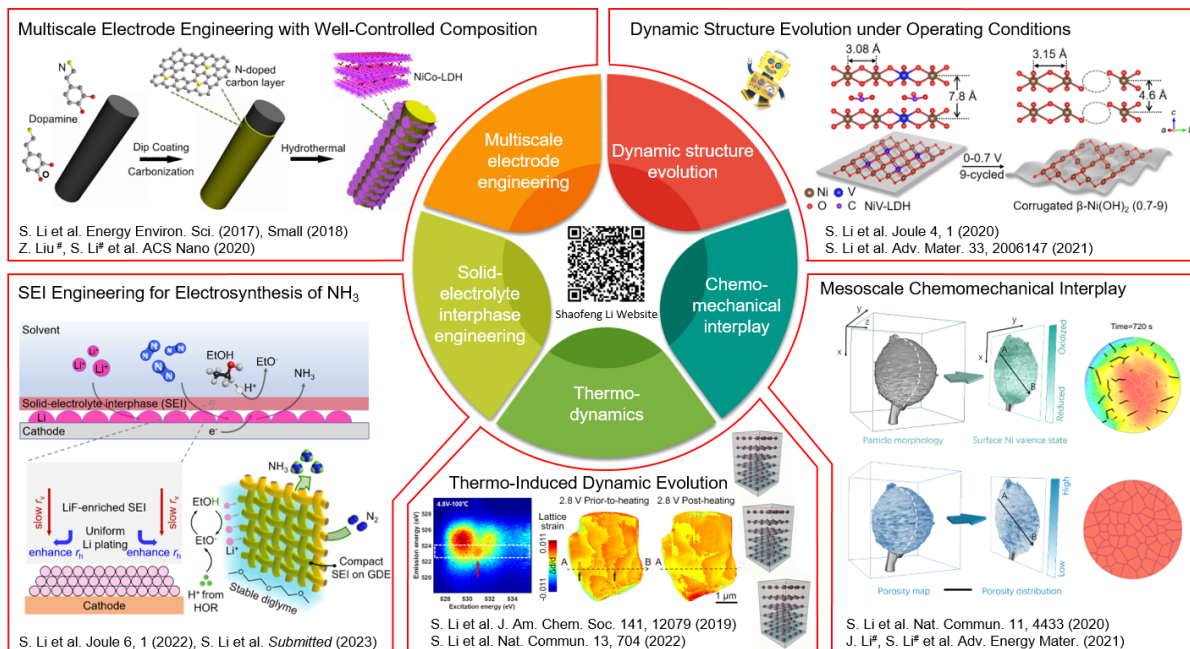
Shaofeng Li^{1,2}, Yijin Liu², Jens K. Nørskov¹, Ib Chorkendorff¹

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²Stanford University, United States

Unveiling the genuine active sites of electrode materials or catalysts under realistic operating conditions holds the key to its practical applications for energy storage and conversion. In this talk, I will show some typical examples on different applications, including supercapacitor, Li-ion battery and lithium-mediated ammonia synthesis:

1. How to reveal dynamic reconstruction of metal hydroxide for high-rate energy storage¹, and further inspiring the rational design of high-performance electrode materials by operando tailoring the defects and strains².
2. How to uncover the surface-to-bulk redox coupling³ and the interplay of the surface chemistry and the bulk microstructure⁴ for layered oxide battery cathode, and further develop strategies for defect and lattice strain modulation⁵.
3. How to disclose the dynamic evolution of the solid-electrolyte interphases (SEI) for Li-mediated ammonia synthesis, and further achieving high selectivity and high rate by combing SEI and electrode engineering⁶.



References

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MOF GLASS BASED SOLID-STATE POLYMER ELECTROLYTE FOR LITHIUM METAL BATTERIES

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Polymer solid-state electrolytes are promising candidates for solid-state lithium metal batteries, but fillers play a very critical role in adjusting their network structure, electrochemical properties, thermal stability, and mechanical properties. However, most of the fillers reported so far are anisotropic, which limits the potential to enable isotropic ion transport. Here, we prepare polyethylene oxide (PEO) based solid-state electrolytes using a metal-organic framework (MOF) glass (namely ZIF-62 glass) as an isotropic functional filler. Calorimetric and diffusion kinetics tests show that the MOF glass addition reduces the glass transition temperature of the polymer phase, improving the mobility of the polymer chains, and thereby facilitating Li-ion transport. By also incorporating a lithium salt (LiTFSI) and ionic liquid (IL), Li-Li symmetric cell tests of the PEO-LiTFSI-MOF glass-IL electrolyte reveal low overpotential, indicating low interfacial impedance. Molecular dynamics simulations show that the isotropic structure of the MOF glass facilitates wettability of the ionic liquid by enhancing interfacial interactions, leading to a less confined ionic liquid structure that promotes Li-ion mobility. Finally, the PEO-LiTFSI-MOF glass-IL electrolyte is used to construct Li-Li iron phosphate full batteries that feature high cycle stability and rate capability.

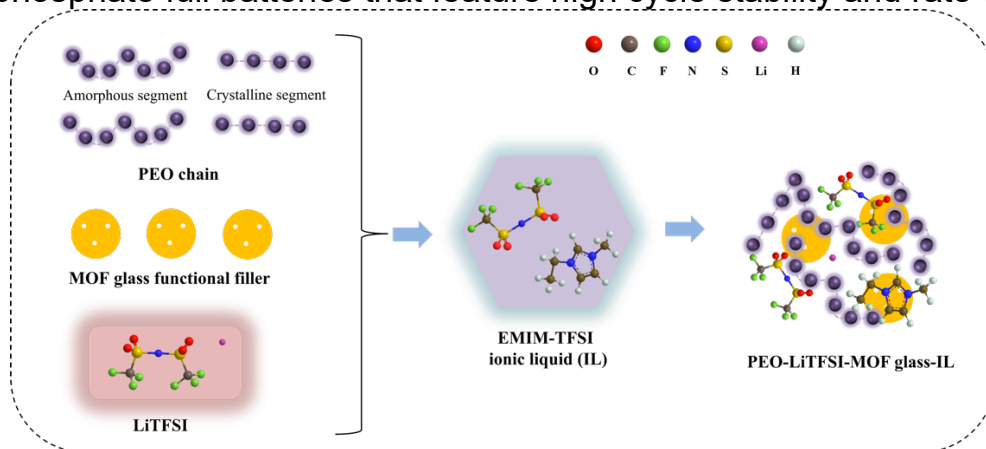


Figure 1. Schematic diagram of the preparation of MOF glass functional filler based solid-state polymer electrolytes with IL.

Keywords: MOF glass, functional filler, solid-state polymer electrolyte, ionic liquid, lithium metal batteries



POLYSTYRENE-*B*-POLY(ETHYLENE-CO-BUTYLENE)-*B*- POLYSTYRENE (SEBS) BASED BIPOLAR MEMBRANE FOR REVERSE-BIAS MODE ENERGY CONVERSION SYSTEM

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Bipolar membranes have drawn attention in energy conversion systems due to its unique function to dissociate or recombine water at its interfacial layer.^[1] BPM under reverse bias evokes a flux of proton and hydroxide ions driven through cation exchange layer (CEL) and anion exchange layer (AEL), respectively. All-hydrocarbon-based BPM can not only mitigate AEL degradation in alkaline environment but also provide alternatives for replacing commonly used perfluorinated CEL.

In this work, elastomer SEBS was chloromethylated to form a common precursor, which was subsequently converted into sulfonated and quaternary ammonium-based SEBS, serving as CEL and AEL of SEBS-based BPM. This divergent route synthesis from the same polymer not only provides a straightforward synthesis path but also allows to control similar properties of both layers (e.g. IEC and functionalized backbone structure). Furthermore, the use of structurally identical backbone for the individual layer was hypothesized to create a miscible junction that contribute to enhance its junction stability. A series of SEBS-derived BPMs with different water dissociation catalyst and individual membrane properties are characterized in a MEA-type water electrolysis cell.

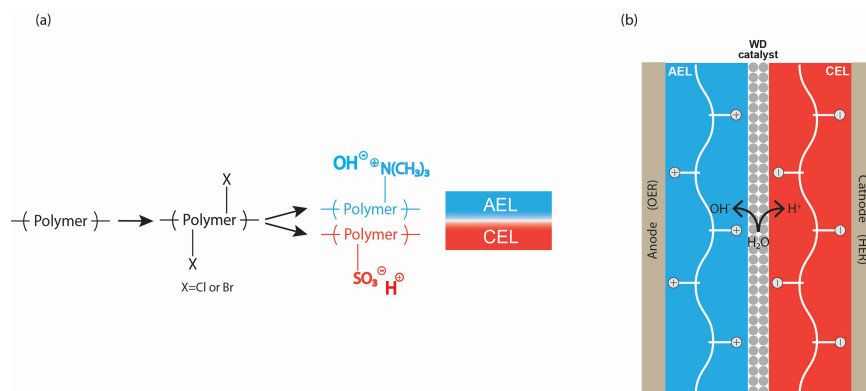


Figure 1. (a) General synthetic route for same backbone BPM (b) BPM in MEA-type cell for water electrolysis

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Oral 5

In-operando investigation of catalysts for oxygen electrocatalysis

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Discovering efficient electrocatalysts is the key to the large-scale adoption of renewable energy technologies such as fuel cells and water electrolysis. Despite the significant progress made in rational design and development of catalyst structures by combined theoretical and experimental approaches, the evolution/degradation of catalyst structures under industrial operating conditions (such as high temperature, corrosive electrolytes, and intermittent operations) is often not taken into account, although it is a decisive factor for the real-world application of the catalysts. Herein, we report our recent findings on the structure evolution/degradation of several types of catalysts—Pt alloys, Ni-based oxides, and Ir-based oxides—for the oxygen reduction and oxygen evolution reactions under industrial conditions, revealed by studies using multiple in-situ/operando electrochemical techniques.



Atomic Scale Simulations of Reactions at Gold-Water Interfaces

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Experimental and computational investigations of reactions at solid-liquid interfaces are challenging due to the presence of the liquid. Computational investigation or electrochemical reactions often neglect the liquid solvent completely, consider a few static solvent configurations, or treat the solvent in the continuum limit. On the other hand, *ab initio* molecular dynamics simulations can, in principle, model reactions with explicit solvent molecules. Here, we report our recent atomic scale computational investigations of reactions at solid-liquid interfaces based on *ab initio* molecular dynamics and machine learning interatomic potentials.

The selectivity of the CO₂ reduction reaction (CO₂RR) has shown remarkable sensitivity to the supporting electrolyte, and several effects of cations on the CO₂RR have been proposed. To understand the possibly different roles of protons and metal cations, we present *ab initio* molecular dynamics calculations of the free energy barriers for CO₂ activation and the competitive adsorption on Au-water interfaces with different concentrations of H⁺ and K⁺ ions. We explore pathways in the CO₂RR and the competing HER at Au(100)-water interfaces with different concentrations of K⁺ and H⁺ ions and find the CO₂ adsorption and the Volmer step to be rate-limiting for the CO₂RR and the HER, respectively.

The free energy barriers to CO₂ adsorption increase as H⁺ replaces K⁺, showing that short-range CO₂-K⁺ interactions are beneficial to CO₂ activation. In contrast, the free energy barrier for the Volmer step decreases as H⁺ replaces K⁺. These changes in the Volmer barrier are correlated to changes in the hydrogen bonding network. However, *ab initio* molecular dynamics simulations are limited by the high computational cost, typically limiting simulations to some picoseconds, which makes it challenging to ensure sampling of the relevant liquid structures.

Machine learning potentials (MLPs) trained to density functional theory calculations can be 5-6 orders of magnitude faster than *ab initio* calculations at a similar accuracy, and we show how it is possible to extend the accessible timescale for reactive events at solid-liquid interfaces from picoseconds to nanoseconds. Using meta-dynamics with path collective variables, we calculate dissociation pathways and two-dimensional free energy surfaces for O₂ dissociation to obtain insight into the structural sensitivity of O₂ activation.



Electrochemical Nitrogen Activation for Ammonia Synthesis

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Ammonia (NH₃) is an important chemical for society to produce fertilizers, pharmaceuticals, polymers, and other chemicals. Electrochemical ammonia synthesis is regarded as a promising route to complement the Haber-Bosch process for the distributed production of fertilizers in small-scale devices powered by renewable electricity.^[1] After rigorous quantitative (*i.e.* gas purification and quantitative isotope measurements) investigations, lithium-mediated nitrogen reduction reaction (Li-NRR) was validated as a promising route for electrochemical ammonia synthesis.^[2,3] Although significant progress has been made to achieve high FE and current density^[4,5], most Li-NRR studies have the limitations of sacrificing solvent as protons for ammonia synthesis and difficulties in scaling up production in batch-type electrochemical cells (*i.e.*, one-compartment cells and autoclaves).

We introduced hydrogen oxidation reaction (HOR) on the anode to provide a sustainable hydrogen source for ammonia synthesis rather than sacrificing solvent as protons.^[6] We here show that the classical catalyst Pt does not work for stable HOR (deactivated in a few minutes) in the organic electrolyte, while PtAu alloy is essential for reducing the anode potential (anode potential: 0.6 V, cell voltage: 4.3 V) avoiding the decremental decomposition of the organic electrolyte. The PtAu alloy demonstrated long-term stability and high activity of HOR in the Li-NRR organic system. *Operando* mass spectrometry of deuterium (D₂) oxidation demonstrated that hydrogen oxidation can continuously provide protons for ammonia synthesis and confirmed the recyclability of ethanol as a proton shuttle. Benefitting from the robust PtAu anode catalysts, the potential cycling method and trade-off strategy of the proton/nitrogen limited region, record high faradaic efficiency of up to 61% and energy efficiency of 13% were achieved at 1 bar of nitrogen.

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Rationalizing the Electrochemistry of Multistep Reactions in General and the HOR/HER on Platinum in Particular

Oral presentation

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In most reactions in electrocatalysis multiple electrons are transferred. Due to the unlikely event of the transfer of more than one electron at once, such reactions are multistep reactions. However, the literature focuses heavily on the one-electron one-step reaction and there seem to be no consensus on how to treat multistep reactions or if the Butler-Volmer model can even be applied.

Here, I will elucidate how such reactions can be treated in a straightforward manner using the Butler-Volmer model. In this process we found that the Tafel slope, despite common practice and a recent IUPAC report, cannot be used to determine the reaction mechanism, as this idea originates from an erroneous derivation in fundamental literature. I continue to explain that also exchange current densities cannot be universally defined for multistep reactions and their value depends on the method chosen in their determination.

Eventually I explain that the HOR/HER mechanism must follow the Heyrovský-Volmer rather than the Tafel-Volmer path on platinum and how errors in the electrochemical analysis have prevented its identification. Finally, I explain how a misunderstanding of the Koutecký-Levich equation has led to a flawed analysis of the pH-dependency of the HOR/HER and how it is impossible to accurately measure its kinetics in half-cells below a pH-value of 11-12 and that the pH-dependency of the HOR/HER as such is perfectly reasonable.

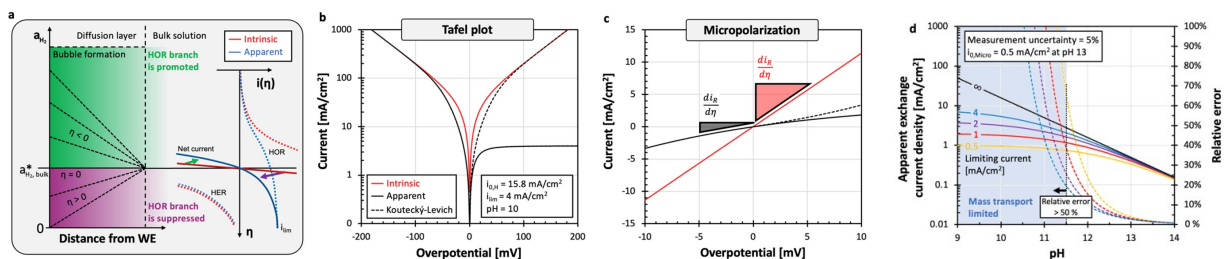


Fig 1 | Mass transport limitations at pH 10. (a) Situation on the electrode. (b) Tafel plot with a Koutecký-Levich correction. (c) Micropolarization with the apparent and intrinsic slope. (d) Measurement errors depending on the pH-value.



Oral 9

Exploring the Activity-Stability Landscape of $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ ($x = 0\text{-}0.33$) for the Oxygen Evolution Reaction at Industrially Relevant Alkaline Electrolysis Conditions

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Developing an efficient and robust electrocatalyst for the oxygen evolution reaction (OER) that is free from scarce raw materials is of paramount importance for the sustainable production of green chemicals and fuels. Significant efforts have been devoted to improving the activity of OER electrocatalysts, while their robustness has been less dwelled upon.¹ Even for $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$, which is known to be one of the most active transition metal-based OER electrocatalysts in alkaline media, its long-term stability under industrially relevant conditions remains questionable. The stability of $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ is known to depend on operating conditions (overpotential, current density, temperature), electrolyte composition (pH, type, and concentration of cations), and its structural and chemical characteristics (diameter and thickness of platelets, intercalating anions, orientation, composition, point and extended defects). Recent studies have shown that the stability of $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ can be improved by inducing cationic vacancies, exfoliation into single layer nanosheets, and by sustaining a dynamic equilibrium with Fe species in the electrolyte.^{2,3} Though these studies have shown improvement in the long-term stability of $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ at mild operating conditions, its stability is expected to aggravate when operated at industrially intensive conditions. In this contribution we report the activity and stability of $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ ($x = 0\text{-}0.33$) for OER in 1, 6, or 10 M KOH, at 75 °C and 10-400 mA/cm² by employing long-term testing over a period of 30 days, supplemented by *operando* Raman investigations at similar conditions. We expect this study to help guide the future design and industrial uptake of advanced $\text{Ni}_{1-x}\text{Fe}_x\text{-LDH}$ based electrodes for OER in alkaline environment.

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MECHANICAL ALLOYING OF NICKEL-BASED CATALYSTS FOR ALKALINE WATER ELECTROLYSIS

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Alkaline water electrolysis is a mature technology and currently undergoing large scale industrialization. Electrodes based on nickel coated steel plates are robust and economical. However, the technology generally operates with low current densities, leading to research in catalyst synthesis, electrode modification, and stack design. Highly efficient, durable, and low-cost catalyst powders, which can be quickly coated on the conventional perforated electrodes is therefore of great interest.

Mechanical alloying was studied to produce nickel-based alloys with high yield. Results show that Ni_2Al_3 and NiAl_3 are dominant phases in the final product after milling Ni and Al powders for 2.25 hours. The found milling profile is applicable to synthesize other catalyst compositions with high product yield ($\geq 95\%$).

The catalyst products were characterized by XRD, SEM and EDX, and deposited on Ni plate electrodes by airbrushing. Following an activation procedure, catalytic performance was evaluated in half-cell electrochemical measurements.

The project is performed in close collaboration with the company Stiesdal Hydrogen A/S.



Oral 11

IDENTIFICATION AND QUANTIFICATION OF DEGRADATION IN COMMERCIAL SOLID OXIDE ELECTROLYSIS STACKS USING THE POWER OF ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

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Electrochemical impedance spectroscopy (EIS) is a powerful diagnostic tool used in a wide range of applications, including solid oxide electrolysis cells (SOECs). While EIS measurements on single-cell level are widely used today, implementation of EIS on stack level is still limited, primarily due to the low impedance of large-footprint cells, which imposes stringent demands on the experimental setup and equipment. In addition, the reported stack-level EIS data in the literature are rarely subjected to detailed analysis through equivalent circuit modeling, thereby limiting the conclusions drawn from such stack impedance measurements.

In this work, we present a case where electrochemical impedance spectroscopy (EIS) on stack level enabled the identification of degradation and failure mechanisms in a commercial 75-cell solid oxide electrolysis cell (SOEC) stack from Topsoe. A defective stack, which did not meet quality control specifications, was subjected to EIS in a blind test. The type of defects present in the stack was not known a priori. The experiment's purpose was to show the potential of using EIS on a stack level to identify degradation mechanisms. A suitable equivalent circuit model was applied and fitted to the EIS data, which enabled the identification of which electrochemical contribution(s) caused the overall degradation of the stack. Additionally, the data was plotted in a degradation space format, which further strengthened the identification of the cause of degradation. This study explores and utilizes the potential of advanced EIS and analysis; and thereby successfully identifies some of the degradation and failure mechanisms taking place in the SOEC stack. This detailed type of degradation analysis has, to the best of knowledge, not previously reported from other groups on commercial stack level. The presented results have convinced Topsoe that EIS on stack levels enables detailed insight into the black box of SOEC stacks, hence a short outlook on Topsoe's strategy to use stack-level EIS even further will be given at the end of the presentation.



Zinc triggers favorable hydrogenation reactions of air electrodes in protonic ceramic cell

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Reversible protonic ceramic cells (RPCCs) show promising performance at intermediate temperatures due to their fast proton transport kinetics. However, their output performance is limited by the sluggish air electrode reactions. Developing materials concurrently conducting protons/oxygen-ions/electrons has been proven to enlarge the air electrode reactive zone and ultimately enhance the electrochemical performance.¹ Cobalt-based perovskite materials, widely used as air electrodes for their great catalytic activity, typically exhibit very low proton uptake capacity. In this work, we introduce zinc into cobalt-based $\text{PrBaCo}_2\text{O}_{5+\delta}$ ($\text{PrBaCo}_{1.9}\text{Zn}_{0.1}\text{O}_{5+\delta}$, PBCZn) to enhance its proton uptake ability. The full cell with PBCZn electrode demonstrated excellent electrochemical performance of 655 mW cm^{-2} at $650 \text{ }^\circ\text{C}$ and a stable operation of 100 hours. The improved proton uptake ability and promising catalytic performance account for such electrochemical performance.

Acknowledgment

This work was financially supported by the Villum Fonden via the project “One-step synthesis of green ammonia from renewables” (no. 35935) as part of the Villum Experimental Program. The first author was funded by a fellowship by the Marie Skłodowska Curie Grants (MSCA) under the Horizon Europe Program HORIZON-TMA-MSCA-PF-EF (Project no.101064064).

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Abstracts – Poster presentations



Phosphorus Recovery and Heavy Metal Removal from Lake Sediments Using Electrodialysis

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Background: Phosphorus (P), although an essential nutrient, is a pollutant when found in excess quantities. Similarly, heavy metals, even though present in very small quantities, are still toxic and extremely harmful to the environment. These pollutants, when available in the lake, are found to be settled in the sediments and get released in the overlying water under anoxic conditions. Electro-dialytic (ED) remediation allows the simultaneous removal of heavy metals and the recovery of phosphorus (P) from sewage sludge ash, municipal wastewater sludge, and harbour sediments^{1,2,3}. This study investigated the performance of 3-compartment (3C) and 2-compartment (2C) ED cells for the simultaneous removal of heavy metals and recovery of P from lake sediments. The sediments were collected from two different lakes in Denmark, Lake Ormstrup (Jutland) and Raadvad Lake (Zealand).

Results: A 3-compartment and 2-compartment batch setups with ion exchange membranes were used for electro-dialytic treatment. After 12 days of the treatment, P recovery was found to be 57% and 42% for Ormstrup and Raadvad sediments, respectively, using a 3-compartment setup; and 33% and 30% using a 2-compartment setup, from Ormstrup and Raadvad sediments, respectively. Cadmium (Cd) and Zinc (Zn) recovery was 78% and 92% from Ormstrup sediment and 73% and 87% from Raadvad sediment using a 3C cell. Using a 2C cell, 69% Cd and 88% Zn were recovered from Ormstrup sediment, and 70% and 89% were recovered from Raadvad Sediment.

Conclusion: A 3-compartment electro-dialytic cell has a better recovery efficiency than a 2-compartment cell. Optimizing treatment parameters (duration, current, stirring velocity) is necessary for enhancing P recovery and heavy metal removal. Since heavy metals and P are recovered in different solutions, the recovered P solution has the potential to be used as a fertilizer.

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Poster 2

SELECTIVE REMOVAL OF PHOSPHORUS FROM WASTEWATER USING AN FE-ACC ELECTRODE IN CDI TECHNOLOGY

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About 70% of the lakes in Denmark do not meet EU Water Framework Directive (WFD) due to the historical build-up of phosphorus in the lake sediments. Capacitive deionisation (CDI) is a promising technology for treating water with low to moderate salt concentrations. CDI operates based on the electric potential across a pair of porous electrodes to remove ions from water through electrostatic attraction and adsorption. CDI generally requires less energy compared to some other desalination methods such as reverse osmosis (RO) and distillation, thus making it energy efficient and cost-effective. The electrodes in CDI are of paramount importance for being the key components responsible for selective ion removal from water. Therefore, this work investigates the performance of iron oxide loaded activated carbon cloth (Fe-ACC) as electrode material in selective removal of phosphorous. Herein, two primary aspects were investigated, 1) selective properties of the Fe-ACC electrode, and 2) regeneration of the electrode after exhausted. The Fe-ACC electrode was fabricated by chemical precipitation of iron oxide nanoparticles into the pores and surface of the chemically oxidized ACC. A synthetic solution containing equal concentrations (500 ppm) of H_2PO_4^- and Cl^- ions was used as water matrix for ion removal operation. The process of electrochemical regeneration of the electrode was examined at different pH ranging from 9 to 12. The results showed that the adsorption capacity of 25 mg H_2PO_4^- per gram of electrode material. Furthermore, the results obtained from the regeneration process showed that about 80% of the electrodes' capacity were regenerated at high alkaline condition. However, more than 50% of the electrode's capacity were lost after 5th cycle of operation. In conclusion, this study reveals that Fe-ACC electrode is promising for selective recovery of phosphorous, however the challenge lies in regeneration of the electrode's original capacity.



SOEC and the effect of impurities
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Topsoe is dedicated to becoming the global leader in carbon emission reduction technologies by 2024. They are achieving this by developing a range of energy-efficient solutions that produce sustainable transportation fuels like ammonia, methanol, and hydrogen. With over 80 years of experience in heterogeneous catalysis and its application to industrial chemical processes, Topsoe is now working on developing strong Power-to-X solutions to fuel the transition towards a sustainable chemical industry and energy infrastructure. One of the key technologies for this transition is the solid oxide electrolysis cell (SOEC) technology, which is recognized as the most energy-efficient among electrolysis solutions. Topsoe's expertise in heterogeneous catalysis is also critical in ensuring an effective downstream catalytic conversion of SOEC products (H₂, CO, or syngas) into green fuels and chemicals.

To address climate change at the necessary pace, Topsoe has committed to achieving net-zero greenhouse gas emissions by 2040. To achieve this ambitious goal, a large-scale industrial application of the SOEC technology is required. Accordingly, Topsoe has announced the construction of a SOEC manufacturing facility in Denmark that will produce electrolysis stacks and modules with a capacity of 500 MW per year. The facility is planned to be operational in 2025¹

This poster presentation provides an overview of the significant impurities that need to be considered when constructing a SOEC system, and their impact on the cell's lifetime. To mitigate the effect of impurities, it is crucial to limit their presence in the reactant gas before it enters the stacks. Additionally, the poster delves into the mechanisms of impurities and their influence on the cell.

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An automated testing platform for Power-to-X materials (P2XTEST)

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Over the last decade, the demand in energy, fuels and chemicals is increasing rapidly, while there is an urgent need to tackle the consequences of climate change. For this reason, P2X technologies are becoming a priority in political agendas around the world. Especially, the development of low-temperature P2X technologies has been rapid and very promising. Nevertheless, a crucial link between their development and successful upscaling is testing. Currently, the commercially available testing devices do not offer fast and reliable electrochemical and stability tests under industrial conditions for P2X materials. In the meantime, autonomous systems gain more and more attention, with special focus on modularity, that provides independence and flexibility in testing and data handling. Our group's work aims for a complete testing setup that enables, low-cost and high-accuracy electrochemical testing for commercial activities in the field of low-temperature P2X technologies. In more detail, it is a compact and automated platform that can run standard electrochemical tests for industrial purposes (e.g. typically: pH 0-14, working temperature 0-200 °C, reactant & product flow, high current densities $>100 \text{ mA cm}^{-2}$) and has the potential to be coupled to characterization devices for in-situ tests (X-ray diffraction, Raman and Infrared). It consists of a control unit connected to a testing chamber (cell) and a computer. Our testing platform has the possibility to become a staple in industrial electrochemical testing or move towards modularity and integration to autonomous, industrial laboratories.

Regardless the development path, we are focusing on i) promoting the research and development of materials, ii) provide high-accuracy, reliable, optimized and low-cost testing procedures iii) and offer a complete system with high flexibility and potential modularity.



Fracture toughness and ionic conductivity of lithium borophosphate glassy electrolytes

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The structural origins of the variation in fracture toughness and ionic conductivity of lithium borophosphate ($x\text{Li}_2\text{O}-(100-x)(0.5\text{B}_2\text{O}_3-0.5\text{P}_2\text{O}_5)$) glass electrolytes with varying composition are investigated. We have performed molecular dynamics simulations combined with bond switching, rings statistic, and persistent homology analyses to provide the atomic picture of the disordered structure of these glasses. Fracture toughness has been characterized through single-edge precracked beam measurements and axial tensile simulations. We find that the deformation and fracture behaviors of the electrolytes are governed by bond switching events of boron, which dissipate the strain energy during fracture. The migration of lithium ions in the electrolyte network is facilitated by hopping between superstructural rings, which reflects the important role of medium-range order structure in determining the lithium-ion diffusion in these glasses.



The effect of electroosmotic dewatering on dewaterability and valorization of lake sediments

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1. key words

Electrochemical treatment, moisture distribution, resource recovery

2. Purpose

Dredging eutrophic lake sediments improves water quality but demands effective dewatering for more accessible transport, and resource optimization, notably phosphorus. This study investigates electroosmotic dewatering's potential to dewater and utilize these sediments efficiently.

3. Materials and methods

The sediments sample was obtained from Bagsværd Lake in Copenhagen, Denmark. A constant DC of 20 mA, 40 mA, and 60 mA were applied through two mesh electrodes for 6 h, and 24 h at 20 mA and 40 mA.

4. Results and discussion

The results derived from drying curves demonstrated electroosmotic dewatering's effective reduction of sediments mass by extracting free and parts of interstitial water. Achieving equilibrium among water removal, energy efficiency, and system stability requires optimizing duration and current. The ramifications of Ohmic heating on dewatering efficiency are dual-fold, encompassing positive and negative aspects. Notably, changes in redox potential and temperature predominantly influence dewaterability. Current conditions minimally extract heavy metals or phosphorus from sediments, facilitating eco-friendly disposal of extracted water and versatile reuse of treated sediments.

5. Conclusions and perspectives

This technology is operational simplicity and well-suited for treating dredged sediments. However, for commercial implementation, focusing on enhancing electric energy efficiency and ensuring stability is imperative in future endeavors.

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Poster 7

Cyclodextrin modified hydrogels for mediated enzymatic bioelectrodes

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Mediated electron transfer (MET) is an important mechanism used in enzymatic bioelectrodes for e.g. biosensors and biofuel cells [1-2]. MET relies on the usage of an electron-transfer mediator, typically an artificial compound undergoing a reversible redox process, to mediate the electron transfer between the redox-active enzyme and the electrode surface. Mediators are preferably immobilized onto the electrode with the enzyme to prevent leakage of mediators to the working solution. Covalent grafting has been frequently used to graft mediators to hydrogel polymers, requiring multiple-step functionalization and labor-intensive purification.

We propose to use the hydrophobic cavity of beta-cyclodextrin to load different types of hydrophobic mediators by forming a supramolecular complex between the cyclodextrin and the mediator. Beta-cyclodextrin will be appended on a suitable polymer, which can be drop-cast onto the electrode in form of a hydrogel to form a bioelectrode by co-entrapment of enzymes in the polymer matrix. In this poster presentation, we present the preliminary results of a ferrocene mediated glucose oxidase based electrode that is made using this strategy.

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ELECTROCHEMICAL PERFORMANCE OF SOLID OXIDE CELLS OPERATED IN CO₂ ELECTROLYSIS

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Solid oxide electrolysis cell (SOEC) is a promising technology and has attracted growing interest in Power-to-X applications for converting renewable energies such as wind or solar into CO₂-neutral chemicals. So far most of the studies were focused on the steam electrolysis or co-electrolysis of steam and CO₂. Only a few studies were devoted to pure CO₂ reduction in SOECs. CO₂ electrolysis not only plays a role in reducing greenhouse gas (GHG) emissions, but it is also a sustainable and clean way to produce pure CO or synthetic hydrocarbon fuels for the chemical industry.

This work studied the Ni/YSZ-supported planar-type SOEC cells operated under CO₂ electrolysis at different current densities. The cells consist of a Ni/3YSZ support, a Ni/8YSZ active electrode, an 8YSZ electrolyte, a CGO barrier layer, and an LSCF/CGO oxygen electrode. The cells were operated at 800 °C and current densities between 0 and -1.25 A/cm² each for more than 1000 h, with a mixture of CO₂/CO (90/10) fed to the Ni/YSZ electrode compartment. The electrochemical performance of the cells was characterized via electrochemical impedance spectroscopy (EIS). It was found that the cell degradation is originated mainly from the Ni/YSZ fuel electrode. The cell operated at -1.25 A/cm² had the highest degradation rate of 361 mV/kh (27.5%/kh), several times higher than that at -0.75 A/cm² (51 mV/kh) and -1 A/cm² (99 mV/kh). Results from the current work show that further improvement of the Ni/YSZ fuel electrode is needed to reduce cell degradation in CO₂ electrolysis, especially at high current densities.