Norsk Kjemisk Selskap

# 11th National Meeting on Inorganic and Materials Chemistry

## Thon Hotel Oslo Airport 27. – 28. February 2024

**Dear colleagues,**

The NKS-FUM meeting is finally here! We are excited to welcome you to Oslo for this year's event.

The meeting event will be held at Thon Hotel Oslo Airport on the 27th and 28th of February, easily accessible from the airport terminals. Attached to the program you can find a screenshot of how to get there.

Our invited speakers will give talks for 40 minutes including 10 minutes for questions, while contributed talks will be 20 minutes long including 5 minutes for questions.

The poster session will be held for 1.5 hours, and we're happy to inform you that there will be a prize for the best poster and student presentation. The prizes will be sponsored by matriks AS. There will be beverages during the poster session and the dinner sponsored by NORECS AS.

It's worth noting that the Inorganic and Materials Chemistry group of NKS (Norsk Kjemisk Selskap) will hold its annual general assembly before the poster session on Tuesday. The assembly is open to everyone.

We hope you will all have an excellent time at the meeting.

**The Organizing Committee**

**Contact people:**
Ingvild Garmo Nilsson- i.g.nilsson@smn.uio.no
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matriks KJEMISK TEKNOLOGI
https://www.matriks.no/

NORECS
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## Day 1: Tuesday 27.02.2024

* The talks marked in green are eligible for the student presentation award

| | No. | Talk | Name | Institute | Title |
|---|---|---|---|---|---|
| 10:00 | | | Truls Norby | | **Welcome** |
| **Session 1** | | | | | **Chair: David Hall** |
| 10:10 | 1 | invited talk | Ingrid Hallsteinsen | NTNU | Domain control by Pulsed Laser Deposition |
| 10:50 | 2 | invited talk | Jelena Popovic-Neuber | UiS | Electrochemical methods for elucidating ion transport in battery materials |
| 11:30 | 3 | talk | Bo Jiang | UiO | Modeling of Local Atomic Structure in Disordered and Nanostructured Materials |
| 11:50 | 4 | talk | Caren Regine Zeiger | NTNU | Bi Solubility in Tetragonal Tungsten Bronzes |
| 12:10 | **Lunch** | | | | |
| **Session 2** | | | | | **Chair: Mari-Ann Einarsrud** |
| 13:30 | 5 | invited talk | Poul Norby | DTU | Operando/in situ studies of prototype battery cells with X-ray and neutron diffraction |
| 14:10 | 6 | talk | Didrik R. Småbråten | SINTEF | Surface Chemistry and Kinetics of Positrodes for Proton Conducting Ceramic Steam Electrolysis |
| 14:30 | 7 | talk | Jonina Bjorg Gudmundsdottir | UiO | Oxygen Exchange Kinetics on $BaGd_{0.3}La_{0.7}Co_2O_{6-\delta}$ Air/Steam Electrodes for Proton Ceramic Electrochemical Cells |
| 14:50 | **Coffee break** | | | | |
| **Session 3** | | | | | **Chair: Ingrid Hallsteinsen** |
| 15:10 | 8 | invited talk | Anja Olafsen Sjåstad | UiO | Pt-Rh nanoparticles to optimized supported catalysts for $NH_3$ slip catalysis |
| 15:50 | 9 | talk | Marcus Grand Michaelsen | NTNU | Solid Solution Engineering of Plastic Crystals for Thermal Energy Storage |
| 16:10 | **NKS meeting and election of board** | | | | |
| 17:10 | **Poster session** | | | | |
| 18:30 | **Dinner** | | | | |

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## Day 2: Wednesday 28.02.2024

*The talks marked in green are eligible for the student presentation award

| | No. | Talk | Name | Institute | Title |
|---|---|---|---|---|---|
| | | | | **Session 4** | **Chair: Julia Glaum** |
| 9:30 | 10 | invited talk | Andreas Orthaber | Uppsala University | Tailoring reactivity, geometry and electronic structure of polyaromatic hydrocarbons with unsaturated heavier main group motifs |
| 10:10 | 11 | talk | Anders Brennhagen | UiO | Revealing the (de)sodiation mechanisms of Bi-metallates through operando X-ray characterisation |
| 10:30 | 12 | talk | Håkon Andersen | UiO | Kinetic study of novel oxygen carriers for chemical looping for hydrogen production: $Ca_{0.6}La_{0.4}Ti_{0.1}Cr_xMn_{0.9-x}O_{3-\delta}$ (x = 0, 0.3, 0.45 & 0.9) |
| 10:50 | **coffee break** | | | | |
| | | | | **Session 5** | **Chair: Ola Nilsen** |
| 11:10 | 13 | invited talk | Julia Glaum | NTNU | Piezoelectric materials as active biomedical implants – a “two-body problem” |
| 11:50 | 14 | talk | Manjunath Balagopalan | UiO | Structure property correlation in organic ferroelectrics |
| 12:10 | **lunch** | | | | |
| | | | | **Session 6** | **Chair: Truls Norby** |
| 13:30 | 15 | invited talk | Helmer Fjellvåg | UiO | In-situ studies of materials; three examples - zeolites/SAPOs - oxide membranes - battery anodes |
| 14:10 | 16 | talk | Wen Xing | SINTEF | Exploring new solid electrolyte support matrix materials for Molten carbonate fuel cell (MCFC) |
| 14:30 | 17 | talk | Matriks AS / NORECS AS | | Novel advanced scientific instrumentation for inorganic and materials chemistry |
| 15:00 | **Concluding Remarks and Awards for the best poster and student presentations** | | | | |

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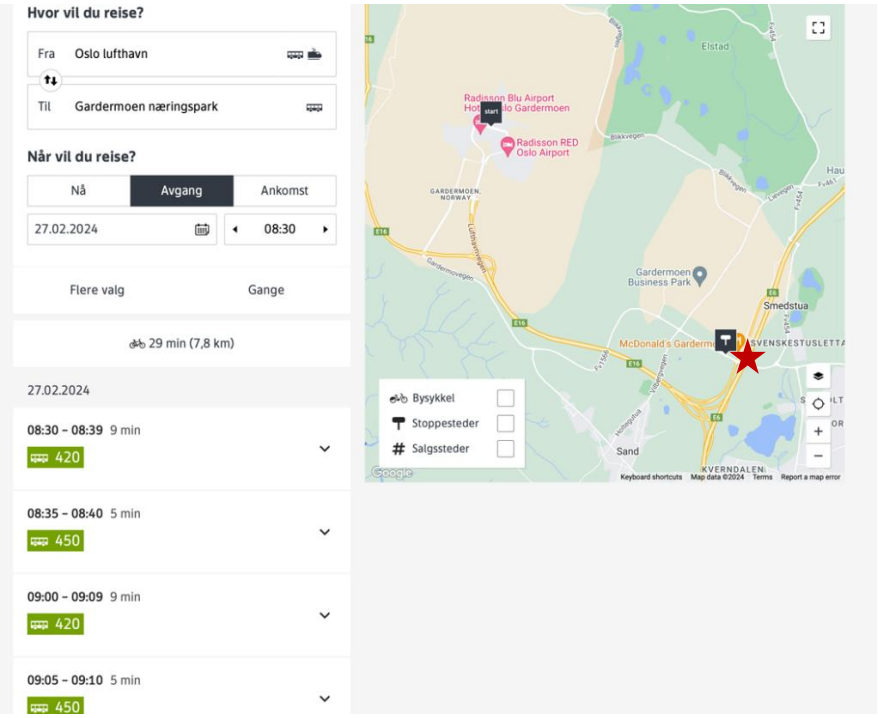
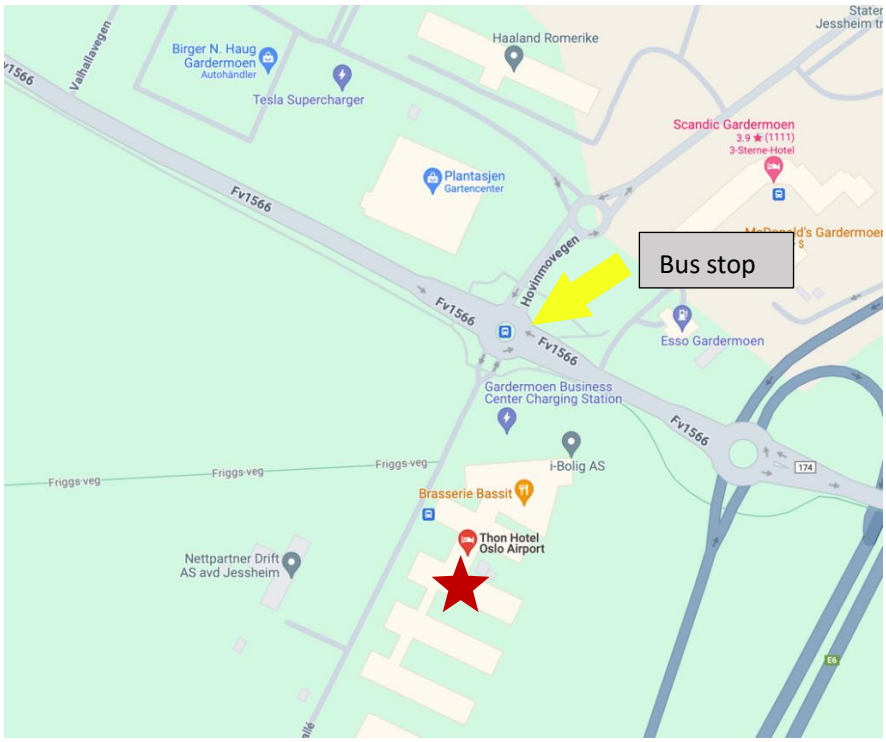
## Connection by public transport from the airport

Connections can be found on: [www.ruter.no](http://www.ruter.no)



# NORECS AS

## Instruments for Inorganic and Materials Chemistry

Materials characterization at high temperatures and controlled atmospheres

## NEW LAUNCHES

### 2Mix

Controls flows of two gases separately or

- ✓ Computer controlled
- ✓ Unlimited user-defined step & ramp programs

**Defaults:**

- Gas A: 0.005 – 50 $ml_n$/min
- Gas B: 0.05 – 500 $ml_n$/min
- Any non-corrosive gas
- Up to 10 bar
- Size: 11 x 20 x 22 cm, 3 kg

**Options&customisation:**

- Corrosive gases
- 20-5000 $l_n$/min
- 20-250 bar
- More MFCs

### 2Wet

- ✓ Adds and evaporates water or other low viscosity fluid to passing gas stream
- ✓ Controls and displays content of evaporated component

**Defaults:**

- 0 to 100% absolute content
- 0 to 100% relative humidity
- Evaporator 150°C
- Heating power 250 W
- 0 to 3 g $H_2O$/min
- Size: 16 x 22 x 27 cm, 5 kg
- Evaporator hose 1.2 m, bend radius 30 cm
- Max pressure: 5 bar

**Options&customisation:**

- Heating power up to 5 kW
- Higher fluid throughput
- Custom static evaporator shapes
- Larger syringe sizes up to 60 g $H_2O$/min
- Higher temperature evaporator

### ProboStat™

- ✓ Electrical characterisation
- ✓ RT — 1600°C
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- ✓ Disk, bar, film, tubular samples
- ✓ New: PEM holder, fixed bed reactor
- ✓ Compatible with all instrumentation

### HumiStat

- ✓ Dynamic mixing of two gases and water vapour
- ✓ Accurate gas dilutions from 20 ppm to 100%
- ✓ Continuous range of water vapour levels from bottle dry gas to pure steam
- ✓ Other evaporating fluids
- ✓ Flow range to 100 $ml_n$/min
- ✓ Other ranges on request

### Furnaces and Ovens

- ✓ From renowned international manufacturers
- ✓ Laboratory and larger scale
- ✓ 80 - 2000°C
- ✓ Air recirculating, vacuum, ashing, etc.
- ✓ Ovens, incubators & drying cabinets
- ✓ Wide variety of chamber sizes
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- ✓ Horizontal or vertical tube
- ✓ Single or three zones
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# ABSTRACTS

## LECTURES

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## Domain engineering by Pulsed Laser Deposition

Y. Liu[1], G. Nordahl[2], S. Boucher[2], K. Kjærnes[3], T. M. Dale[2], R. Chopdekar[4], Arenholz. E[4], Tybell[3], T, M. Nord[2] and I. Hallsteinsen[1]

1 Department of Materials Science and Engineering, NTNU - Norwegian University of Science and Technology, Trondheim, 7491, Norway
2 Department of Physics, NTNU - Norwegian University of Science and Technology, Trondheim, 7491, Norway
2Department of Electronic Systems, NTNU - Norwegian University of Science and Technology, Trondheim, 7491, Norway
4Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA
*Ingrid.hallsteinsen@ntnu.no (Corresponding author and presenter)

Epitaxy is one of the most powerful techniques to fabricate materials while controlling their properties at nanoscale, enabling the development of advanced devices. In this talk I will look at how we use anisotropic strain to control structural domains between different symmetry classes of perovskite oxides. I will focus on the model system $LaFeO_3$, orthorhombic, interfaced with La/$SrMnO_3$ rhombohedral. The thin epitaxial films are made by Pulsed Laser Deposition, and the domain control comes from using different substrates of different symmetries. By using anisotropic strain, we can create mono-domain films which translate also the magnetic properties, in this case antiferromagnetic into monodomain samples, crucial for device development. We use highly sophisticated new STEM techniques including precession (SPED) and higher order laue zones (HOLZ) to image the domains forming, as well as the magnetic domains.

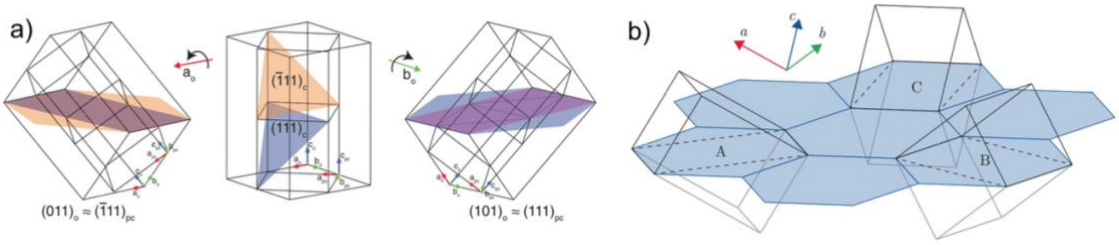



Image courtesy of Kristoffer Kjærnes. a) Relationship of the $(101)_O$ and $(011)_O$ facets with $(111)_{pc}$ and $(111)_{pc}$ crystal planes, respectively. b) Three-fold rotation of the orthorombic unit cell on the $(111)_{pc}$ facet.

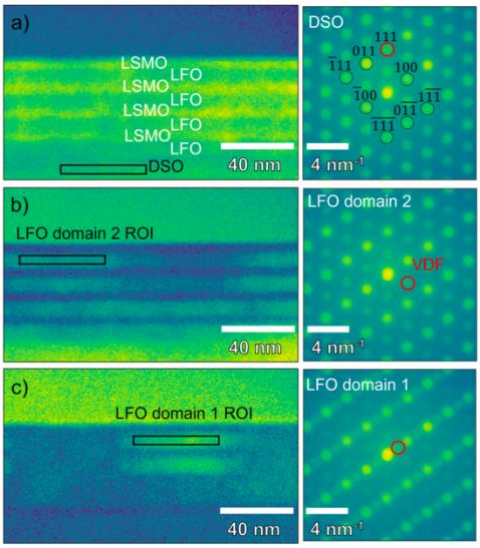



Image courtesy of Susanne Boucher. S-SPED VDF reconstructions of $(LSMO/LFO)_{10}$/STO ac- quired in the $[011]_{pc}$ zone axis with diffraction patterns from regions of interest indicated by with black squares. Red circles indicate diffraction spots used for VDF generation. VDF and diffraction pattern from a) DSO, b) LFO domain 2, c) LFO domain 1.

# Electrochemical methods for elucidating ion transport in battery materials

Jelena Popovic-Neuber

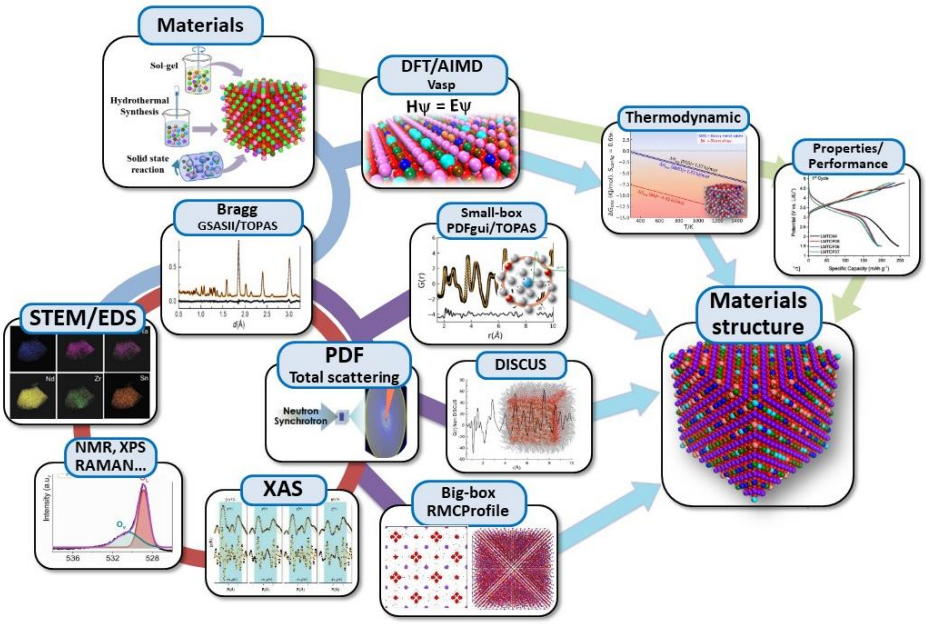
Department of Energy and Petroleum Engineering, University of Stavanger

Advance or development of new battery materials typically involves improvement of properties related to ion transport such as room temperature ionic conductivity, cationic transference numbers and diffusion coefficients. In the first part of my talk, I will introduce some of the most important electrochemical techniques necessary to study these properties, including electrochemical impedance spectroscopy (EIS) and galvanostatic or potentiostatic (intermittent) polarization technique (GITT/PITT). In the second part of my talk, I will show how these techniques were successfully employed to study ion transport mechanisms in battery electrolytes (liquids, thiosulphates), interphases (e.g., solid electrolyte interphases), anodes (carbonaceous materials), and cathodes (ferrophosphates).

# Modeling of Local Atomic Structure in Disordered and Nanostructured Materials

Bo Jiang*[1],
[1]Department of Chemistry, Centre for Materials Science and Nanotechnology, University of Oslo.

**Abstract:**
It is widely recognized the understanding of local atomic structure of complex materials (such as those used in energy storage, catalysis, and a wide array of other functional materials) remains a challenge challenging due to limited experimental observation tools. The unique properties and characteristics of complex materials are governed by these intricate structural-chemical relationships. Pair distribution functions (PDF) obtained from total scattering (high energy synchrotron X-ray and Neutron scattering) can reveal both the local and intermediate range structure of crystalline and disordered materials, especially the local distortions and structural coherence up to several tens of Ångstrøm. A combination of multiple approaches and software using *STEM-EDS*, *PDFgui, TOPAS v6*, DISCUS and *RMCProfile* (Reverse Monte Carlo software) were used for characterizing disordered and nanostructured materials through synchrotron X-ray, neutron total scattering characterization and related probes methods, such as X-ray absorption spectroscopy (XAS), NMR, XPS, RAMAN et, al. The experimental activity is closely supported by density functional theory (DFT) and *ab* initio molecular dynamics (AIMD) simulations to provide a comprehensive understanding.[1-4]

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*boji@uio.no, https://scholar.google.no/citations?user=8cRJIe4AAAAJ&hl=en/

# Bi Solubility in Tetragonal Tungsten Bronzes

*Caren Regine Zeiger, Benjamin Albert Dobson Williamson, Julian Walker, Mari-Ann Einarsrud, and Tor Grande**

Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

**ABSTRACT**

The ferroelectric tetragonal tungsten bronze (TTB) $Pb_5Nb_{10}O_{30}$ (PN) forms morphotropic phase boundaries (MPBs) when in solid solution with other TTBs. However, as PN contains lead, the advancement of a similarly potent but lead-free TTB based on Bi could boost lead-free TTB MPB systems. One potential candidate was identified in the TTB $K_4Bi_2Nb_{10}O_{30}$ (KBN), however it was recently found to have a centrosymmetric crystal structure. We therefore investigated whether ferroelectricity could be induced into KBN by increasing its $Bi^{3+}$ content and synthesised 13 compositions with Bi-content above two $Bi^{3+}$ per unit cell. The modified solid state synthesis routes aimed to charge balance higher Bi-contents by either introducing more cation vacancies or substitute lower valent B-site cations. In the resulting analysis, an additional pyrochlore phase was found for almost every examined composition. First-principles calculations combined with chemical considerations as well as the tolerance factor were used as tools in order to understand the instability of the TTB structure at increased Bi-contents. As $Bi^{3+}$ cannot fully replace $Pb^{2+}$ in ferroelectric TTBs, we determined that Bi-rich TTBs are unlikely to develop in-plane polarisation similar to the mechanism found in PN.

**Operando/in situ studies of prototype battery cells with X-ray and neutron diffraction**

Poul Norby

# Surface Chemistry and Kinetics of Positrodes for Proton Conducting Ceramic Steam Electrolysis

Didrik R. Småbråten

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Proton conducting ceramic steam electrolysis (PCCEL) represent an emerging technology for cost-efficient stationary energy storage, power generation and fuel production with excellent electrical efficiency. One of the main challenges of intermediate temperature operation of PCCEL is the limitations on the positrode kinetics. The underlying mechanisms that govern the electrode kinetics are however yet fully understood. To develop high-performance PCCEL systems it is therefore imperative to further improve our understanding of the positrode kinetics. However, due to an intricate coupling between the surface kinetics, surface chemistry, and operating conditions, experimentally decoupling the different contributions to the electrochemical performance becomes a non-trivial task.

Atomistic modelling using Density Functional Theory (DFT) calculations is a valuable tool to study such intricately coupled phenomena; complex transport or reaction processes are broken down to their most elementary steps, and the surface chemistry is fully controlled. The rate limiting step that governs the electrode kinetics at relevant operating conditions can hence be determined. Here, we present our recent progress on DFT modelling of the surface chemistry and kinetics of positrodes for PCCEL. We first discuss a 1D mechanism to describe the transport processes at the electrode surface during steam electrolysis. Next, we discuss the DFT methodology used to determine surface thermodynamics and surface kinetics. Finally, we evaluate the thermodynamics and kinetics for relevant processes on different model surfaces.

Acknowledgements
**FME HYDROGENi** is financed by its industry partners and the Norwegian government through the Norwegian Research Council's Centres for Environment-friendly Energy Research programme (FMETEKN, project no. 333118). Computational resources were provided by Sigma2 (project no. NN19259K).

# Oxygen Exchange Kinetics of $BaGd_{0.3}La_{0.7}Co_2O_{6-\delta}$ Air/Steam Electrode for Proton Ceramic Electrochemical Cells

**J.B. Guðmundsdóttir[1], E. Vøllestad[2], R. Haugsrud[1], J.M. Polfus[1]**

[1]*Department of Chemistry, SMN, University of Oslo, Gaustadalléen 21, 0349 Oslo, Norway*

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Proton ceramic electrochemical cells (PCECs) show promise for cost-efficient steam electrolysis, power generation, and membrane reactors. However, the air/steam electrode is a restricting factor in their performance, with the oxygen evolution and reduction reactions being rate limiting. A mechanistic understanding of the reaction steps at the electrodes is therefore required to further develop high-performance electrodes and cell architectures.

Pulsed Isotope Exchange (PIE) is a gas phase analysis method that allows for fast characterisation of the oxygen surface exchange rate of powder samples [1]. The surface exchange of oxygen is measured as a function of oxygen pressure and temperature, as well as the effect of water on the exchange rate. The reaction mechanisms and rate determining steps are investigated further by electrochemical impedance spectroscopy on model electrodes at temperatures from 500 °C down to 200°C in different $pO_2$s and $pH_2O$s.

Various compositions of $Ba_{1-x}Gd_{0.8-y}La_{0.2+x+y}Co_2O_{6-\delta}$, which are double perovskite type materials, have been shown to be efficient triple conducting air/steam electrodes for PCECs at intermediate temperatures [2, 3]. $BaGd_{0.3}La_{0.7}Co_2O_{6-\delta}$ shows an oxygen exchange limited by dissociative adsorption in all measured $pO_2$s with activation energies ranging from 0.8 eV to 1.1 eV in dry atmospheres, which is comparable to other double perovskite cobaltites [4, 5]. While the presence of water does not change the rate limiting step, it lowers the exchange rate and increases the activation energy in high $pO_2$ and increases the exchange rate and lowers the activation energy in low $pO_2$s. Electrochemical impedance measurements show similar activation energies to PIE in the same atmospheres and temperature range.

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# Pt-Rh nanoparticles to optimize supported catalysts for $NH_3$ slip catalysis

Anja Olafsen Sjåstad and Martin Jensen

Center for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo,

P.O. Box 1033 Blindern, N-0315 Oslo, Norway

Abatement processes for ammonia ($NH_3$) slip are subject to renewed interest, as new technologies for using liquid $NH_3$ as fuel in the maritime sector gain huge attention. One such technology is selective oxidation of $NH_3$ to nitrogen ($N_2$).

This talk will discuss several aspects on the synthesis of well-defined Pt-Rh nanoparticles and the conversion of them into $Al_2O_3$-supported mono- and bimetallic Pt-Rh model catalysts. Key materials parameters explored are nanoparticle size, degree of alloying and element distribution as well as the stable element configuration at $NH_3$ slip conditions. Additionally, the talk will provide results from the catalytic performance tests performed in a fixed bed reactor between 180 – 400 °C in 1000 ppm $NH_3$, 5% $O_2$ in $N_2$ at a gas velocity of 1 200 000 $h^{-1}$. Our results point to that enhanced catalytic performance is obtained for alloyed nanoparticles, with Rh decorating the surface to promote $N_2$ selectivity with presence of Pt to accelerate the catalytic activity. The talk will conclude with some in-situ TEM results on the stability of bimetallic Pt-Rh nanoparticles and some perspectives on how to refine the element distribution in the particles to further enhance their performance.

This talk is based on parts of the PhD work of Martin Jensen with contributions from the authors given in references 1-5.

**References**

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# Solid Solution Engineering of Plastic Crystals for Thermal Energy Storage

Marcus Grand Michaelsen

*Department of Materials Science and Engineering, Norwegian University of Science and Technology*

Increasing the share of renewable energy sources in global energy production is a major challenge for the green energy transition. In particular, the intermittent nature of renewable energy sources such as wind and solar power, poses challenges related to offsets between periods of supply and demand. Thermal Energy Storage (TES) is recognized as a promising technology for mitigating challenges with intermittent energy sources.[1] In past decades, attention has been given to solid-liquid Phase–Change Materials (PCMs), aiming to store excess thermal energy from renewable energy sources by utilizing the latent heat in the phase transitions of materials. Recently, the concept of solid–solid PCMs has gained some attention due to advantages of smaller volume changes and no liquid formation.[2] Here, we present a study of Plastic Crystals (PCs),[3] a class of material displaying solid–solid, order–disorder phase transitions with high entropy changes, as candidate materials for PCMs. The $[N(C_3H_7)_4]_x[N(C_4H_9)_4]_{1-x}[FeBrCl_3]$ binary system has been studied using in-situ Synchrotron X-ray Diffraction and Differential Scanning Calorimetry in order to evaluate the effect of compositional changes on the relationship between transition temperature, enthalpy, structure and molecular composition. The system was chosen in order to study the specific effects of cation size in molecular ionic plastic crystals. Our study shows that a limited region of partial solid solution is achieved for $x < 0.5$, where the solid–solid phase transition temperature and entropy of transition varies continuously with the the mole fraction $x$ of the solid solution. The nature of the solid solubility is discussed.

[1] Abraham Alem Kebede et al. "A comprehensive review of stationary energy storage devices for large scale renewable energy sources grid integration". In: *Renewable and Sustainable Energy Reviews* 159 (2022). ISSN: 13640321. DOI: 10.1016/j.rser.2022.112213.

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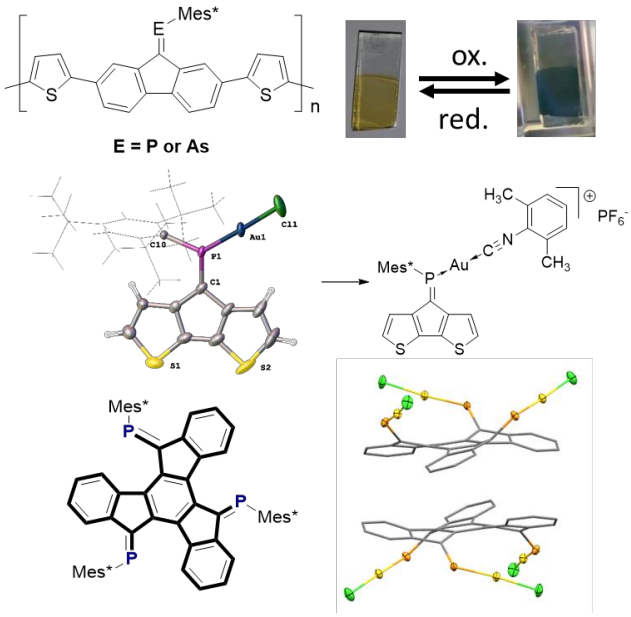
**Tailoring reactivity, geometry and electronic structure of polyaromatic hydrocarbons with unsaturated heavier main group motifs**

*Andreas Orthaber, Uppsala University*

Research into the heavier group 15 alkenes, e.g. phosphaalkenes, originated from a curiosity driven challenge to overcome the empirical double bond rule, inferring instability of these isolobal “alkene” analogues. With suitable approaches of thermodynamic and kinetic stabilisation such “P=C” and “As=C” containing systems can be realized, and their fascinating bonding situation can be utilized to go beyond the boundaries of organic functionalisation to tailor opto-electronic properties of PAHs, by judicious elemental substitution. We present examples of heterofulvenoidal and heteroquinoidal motifs as functional materials for opto-electronic applications. Their highly tunable and modular redox-reactivity and optical properties are also explored towards molecular motion, supramolecular chemistry and other reactivity studies.




Examples of fluorene, cyclopentaditiophene and truxene-based pnictaalkenes.

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# Revealing the desodiation mechanisms of Bi-metallates through *operando* X-ray characterisation

A. Brennhagen, C. Skautvedt, Amalie Skurtveit, C. Cavallo, D.S. Wragg, P. Vajeeston, A.O. Sjåstad, A.Y. Koposov, and H. Fjellvåg

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Na-ion batteries is entering the battery market as an alternative to Li-ion batteries. To improve their overall performance it is crucial to develop new types of anode materials with high capacity and long cycle life. Materials combing conversion and alloying mechanisms (CAMs) are promising anodes with their high capacity, but obtaining good cycling stability is still challenging. A comprehensive understanding of the cycling and degradation mechanism of these materials is crucial to improve their performance.

Bi-metallates, with a general formula of Bi−TM−O (TM = transition metal) is a group of ternary CAMs. Their general cycling mechanism consists of an irreversible conversion reaction forming nanoparticles of Bi-metal embedded in a Na-TM-O matrix during the first sodiation, followed by a reversible two-step alloying reaction forming $Na_3Bi$ with NaBi as an intermediate phase. In this work, we have used *operando* X-ray diffraction (XRD), pair distribution function (PDF) analysis and X-ray absorption spectroscopy (XAS) to investigate the desodiation mechanisms of $Bi_2MoO_6$ and $BiFeO_3$.

Through this work, we discovered that $Bi_2MoO_6$ forms the cubic version of $Na_3Bi$ (c-$Na_3Bi$) while $BiFeO_3$ forms hexagonal $Na_3Bi$ (h-$Na_3Bi$) in addition to c-$Na_3Bi$ during the first sodiation. In the desodiated state, the Bi-particles are partially oxidised, while still maintaining the Bi-metal structure, indicating that it is only the Bi atoms at the interface between the Bi nanoparticles and the Na−TM−O matrix that is oxidised. During cycling the $Na_xBi$ particles grow larger thus increasing the distance between them and increasing the impedance in the material. This is considered to be the main driver for the capacity degradation that was observed during the first 20 cycles. The *operando* XAS data also revealed that $Mo^{6+}$ in $Bi_2MoO_6$ does not change oxidation state during cycling, but changes coordination between tetrahedral and distorted octahedral coordination during cycling. The cycling and degradation mechanisms of $Bi_2MoO_6$ is summarised in Figure 1.

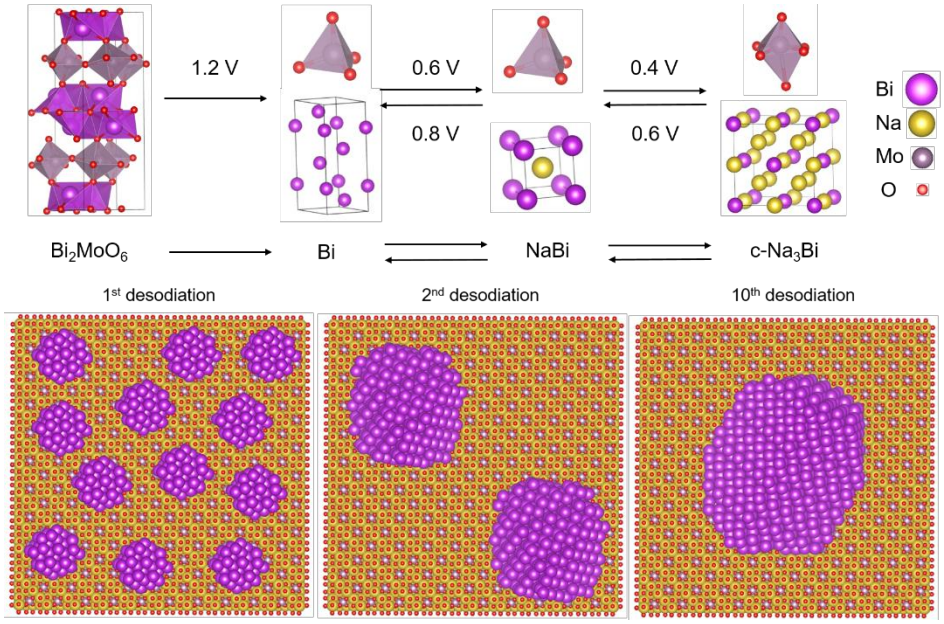


**Figure 1: Graphical illustration of the cycling and degradation mechanism of $Bi_2MoO_6$. The top part illustrates the cycling mechanism where $Bi_2MoO_6$ irreversibly converts into Bi (which further reversibly alloys to NaBi and $Na_3Bi$) in a Na−Mo−O matrix with tetrahedrally coordinated Mo, which further shifts into octahedral coordination. The bottom part is a graphical illustration of the growth of the Bi crystallites with increasing cycle number.**

# Kinetic study of novel oxygen carriers for chemical looping for hydrogen production: $Ca_{0.6}La_{0.4}Ti_{0.1}Cr_xMn_{0.9-x}O_{3-\delta}$ (x = 0, 0.3, 0.45 & 0.9)

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Chemical looping for hydrogen production (CLHP) shows the potential to substantially lower the $CO_2$ emissions from $H_2$ production with hydrocarbon sources[1]. In CLHP, an oxygen-carrying material (OCM) is reduced by a hydrocarbon source to produce syngas, followed by partly oxidation with steam to generate pure $H_2$, before re-oxidation with air to balance the energy demand[2]. However, commercialization of CLHP is still limited by the OCM which should possess a demanding set of properties; catalytic activity towards the red-ox processes without forming coke, sufficient oxygen transport and storage capacity, chemical and microstructural stability over numerous redox cycles, and be abundant with no environmental and societal issues[3].

$Ca/Sr_{1-x}La_xBO_3$ (B = Ti, Cr, Mn, Co, or Fe) perovskites are interesting OCM candidates, showing good chemical stability, high mixed ionic- and electronic conductivity and reversible oxygen stoichiometry over a wide range of reaction conditions[4,5]. In this work, a matrix of $Ca_{0.6}La_{0.4}Ti_{0.1}Cr_xMn_{0.9-x}O_{3-\delta}$, x = 0, 0.3, 0.45 and 0.9, has been studied to investigate the effects of the Cr/Mn content on oxygen exchange kinetic, chemical stability and oxygen stoichiometry.

Pulse Isotope Exchange measurement was utilized to investigate the oxygen exchange of the different compositions as a function of $pO_2$ and temperatures to determine the total oxygen exchange rate ($\Re_0$), as well as, rates for dissociative adsorption ($\Re_a$) and incorporation ($\Re_i$). Chemical stability and oxygen stoichiometry of the different compositions were tested by thermogravimetric analysis under simulated CLHP operating conditions, followed by XRD and SEM.

These novel materials show excellent chemical stability and adequate regenerative oxygen stoichiometry over the whole CLHP range. Variations in the oxygen exchange kinetics and capacity, and the chemical stability, will be discussed with basis in the material's point defect thermodynamics.

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## Acknowledgement

This study was performed as part of the OxHyPro project "Novel oxygen carriers in sustainable hydrogen production ", under the CLIMIT programme; the grant application no. 315083 funded by the Research Council of Norway.

Piezoelectric materials as active biomedical implants – a “two-body problem”

Julia Glaum

Piezoelectric materials are widely used as sensors and actuators, for energy harvesting and vibration control in many industrial and every-day devices. They have established themselves as well in the medical device market as core components in e.g. ultrasound applications and for surgical tools. For *in vivo* applications, this versatile class of materials could similarly enable localized pressure sensing, energy harvesting from muscle motion or stimulation of tissue re-generation after surgery. However, piezoelectric materials have not made the jump into clinical usage so far. The main challenge here is that materials used *in-vivo* have to be biocompatible. This is a concept that goes way beyond simple chemical toxicity but covers all aspects that influence the safe performance of a material at the implant site under the complex conditions that the body imposes.

The investigation and adaption of piezoelectric materials for *in*-vivo applications is a rapidly growing research field that brings together scientists from a wide range of disciplines. Here, we will take an in-depth look into the state of the art of the applicability of piezoelectric materials for *in vivo* biomedical applications. This will be done both from the view of the body as well as from the view of the implant material – as both influence each other. We will investigate the boundary conditions that the body imposes on implant materials in different applications and how these might impact the functionality and stability of piezoelectric implants. And *vice versa* we will explore the influence of material properties, such as surface topography, chemical composition and mechanical properties, on the living system. In that spirit, we will discuss future application areas for this versatile class of materials in the biomedical realm.

# Structure-property correlation in hexamine-based novel organic ferroelectrics

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Organic ferroelectrics have great potential to be used in many practical applications in the fields of Fe-RAM in memory devices, sensors, etc. They have unique characteristics such as light weight, flexibility, non-toxicity, etc., and can be an alternative to the lead-containing ferroelectric.

We have synthesized hexamethylene-based co-crystals, ***HMTAX***, and studied its crystal structure by single crystal XRD confirming a polar space group for the same. We further investigated the structural properties by powder X-ray diffraction (PXRD), Raman spectroscopy, Differential scanning Calorimetry (DSC), etc. Ferroelectric and dielectric measurements were carried out and a detailed structure-property correlation was performed. The compound exhibits a ferroelectric PE hysteresis loop at room temperature. The dielectric spectroscopy of the ***HMTAX*** system shows a dielectric anomaly around 315 K ($T_1$) possibly suggesting its ferroelectric to paraelectric transition. DSC shows an exothermic change around $T_1$. From the Rietveld refinement analysis of the temperature-dependent PXRD data, an anomaly in the lattice parameters is observed around the same temperature where the dielectric anomaly was observed. Temperature-dependent Raman phonon frequencies (FWHM) also show such anomalous behavior at $T_1$, confirming the structural distortion occurring around $T_1$ = 315 K in ***HMTAX***. In this work, we demonstrate how different structural characterization techniques probing different physical properties, can be combined to understand the structure-property correlations in organic ferroelectric materials.

**In-situ studies of materials; three examples - zeolites/sapos - oxide membranes - battery anodes**

Helmer Fjellvåg

# Exploring new solid electrolyte support matrix materials for Molten carbonate fuel cell (MCFC)

Wen Xing[1], Nikolai Gaukas[1], Christelle Denonville[1], Aliaxandr Martsinchyk[2], Jaroslaw Milewski[2], Pavel Shuhayeu[2], Arkadiusz Szczesniak[2], Olaf Dybinski[2], Arkadiusz Piotr Sieńko[3]

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## Abstract

New oxide ion conductors with perovskite structures containing alkaline metal were explored for use as solid support materials for MCFCs (Molten Carbonate Fuel Cells). The conductivity of two candidates, BNT ($0.94Bi_{0.5}Na_{0.5}TiO_3$-$0.06BaTiO_3$) and LNT ($La_{0.5}Na_{0.5}TiO_3$), in an oxidation atmosphere, were measured and compared. The conductivity measurement of BNT in a reducing atmosphere indicated the reduction of BNT to Bi metal by a sharp change in conductivity. It limited the lifetime of the fuel cell using BNT as solid support. Fuel cell measurements using the alternative perovskite LNT showed excellent stability under fuel cell operation conditions and high-power density compared to conventional MCFC with $LiAlO_2$ as the solid matrix. The reason for obtaining high electrochemical performance using the LNT matrix is discussed.

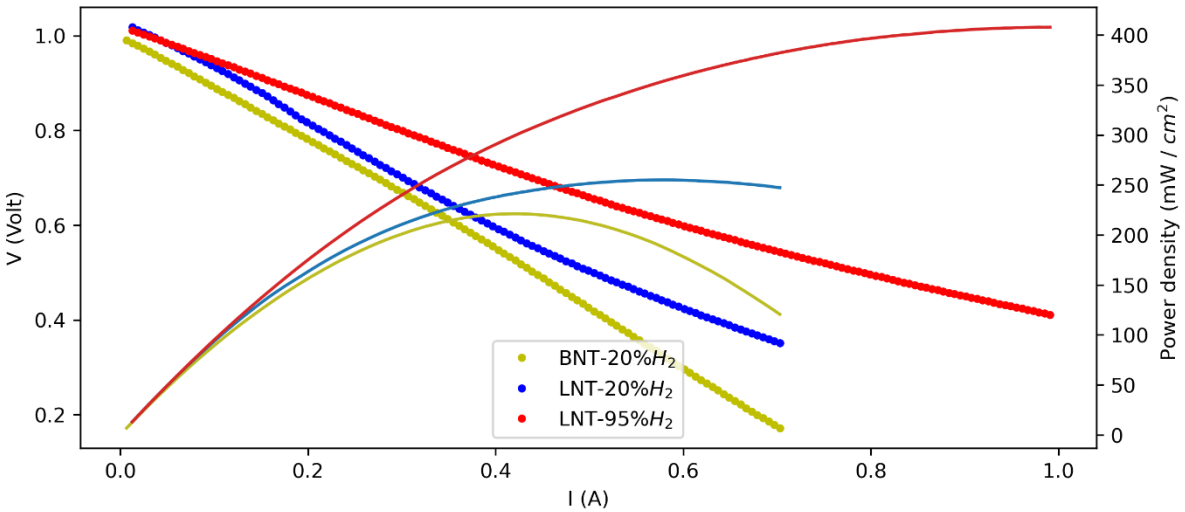


*Figure 1: I-V measurement results and power output for symmetric cells with BNT and LNT solid matrix support with 20% and 95% $H_2$ on the fuel side at 650 °C. The cell area is 1 $cm^2$.*

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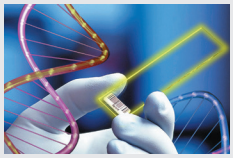

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## POSTERS

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| Poster | Name | Institution | Title |
|---|---|---|---|
| 1 | Jonas Grill | UiS | Electrochemical impedance spectroscopy as a tool to study battery interfaces |
| 2 | Yabing Wen | UiO | Polarization from the space charge layer at the interfaces including grain boundaries and interfaces between Ag electrodes and proton ceramic electrolytes |
| 3 | Anjali Choubey | UiO | Exploring near-earth nickelates as absorber material for tandem solar cell application |
| 4 | Caitlin Guzzo | NTNU | Functional compositional engineering in lead-free piezoelectric bioceramics |
| 5 | Dharsana Pulikkottil Dinesh | UiO | Advancing the application space of barium titanate ($BaTiO_3$) via ALD |
| 6 | Luyang Wang | UiO | Minority bulk and surface proton conduction in ceramic positrodes for proton ceramic electrochemical cells |
| 7 | Stine Roen | UiO | $Ba_{0.95}La_{0.05}(Fe_{0.7}Ni_{0.2}Zn_{0.1})O_{3-\delta}$ as steam electrode in proton ceramic electrochemical cells |
| 8 | Patrick Ewerhardt | UiO | Modelling and characterization of negatrodes in proton ceramic electrochemical cells |
| 9 | Vilde Gahr Sturtzel Lunde | IFE | Machine learning-guided discovery of laves phases for magnetocaloric hydrogen liquefaction |
| 10 | Mengxin Wu | UiO | Performance and degradation of positrodes for proton ceramic electrolysers |
| | Arkalekha Mandal | UiO | Effect of ionic shape and size in dictating piezoelectric property of organic plastic ionic crystals |
| | Truls Norby | UiO | Electrodics for proton ceramic electrochemical cells |
| | Xinwei Sun | UiO | Charge and mass transfer polarization of BGLC37 positrodes for proton ceramic electrochemical cells |

*Posters with numbers are eligible for the student poster award

Electrochemical impedance spectroscopy as a tool to study battery interfaces

Jonas Grill, Jelena Popovic

Department of Energy and Petroleum Engineering, University of Stavanger, Norway

Electrochemical impedance spectroscopy (EIS) is a powerful tool for studying electrochemical systems as it can help deconvolute electrochemical processes in batteries based on their relaxation times, allowing observation of individual processes in-situ and over time[1]. This is especially useful for observations of the SEI (solid electrolyte interface) in batteries, as the SEI plays a crucial role in cell performance and cycle life but is a buried thin layer. With the help of EIS, the evolution of SEI properties such as resistivity and activation energy for ion transport can be measured[2, 3]. By combining results from EIS and additional methods like FIB-SEM (focused ion beam scanning electron miscroscope) and XPS (X-ray photoelectron spectroscopy) for further morphological and chemical analysis, a full picture of SEI can be drawn.

This poster showcases two current research topics concerning SEI evolution in symmetric silicon cells with liquid electrolytes (LP30: 1 M $LiPF_6$ in 50 % v/v ethylene carbonate and 50 % v/v dimethyl carbonate) and potassium cells with the W-doped $K_3SbS_4$ solid-state potassium electrolyte. The main questions to be answered are if SEIs form chemically at other, less reactive electrodes than alkali metals and if the formed SEIs generally stabilize after longer time periods. In the first case, we observe a SEI formation on Si electrodes after multiple days to weeks. In the second case, a stabilization of the SEI is observed after multiple days.

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# Polarization from the space charge layer at the interfaces including grain boundaries and interfaces between Ag electrodes and proton ceramic electrolytes

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## Abstract

Space charge layers are common at heterogeneous interfaces [1]. Previous investigations [2-4] into the space charge layer (scl) effects at the interface between metal electrodes and proton-conducing electrolytes were predominantly done by the Distribution of Relaxation Times (DRT) method due to the challenge of distinguishing between various transfer processes through impedance spectroscopy. In the present study, the presence of a space charge layer at the interface between Ag electrodes and proton-conducting perovskite electrolytes of $BaZr_{0.9}Y_{0.1}O_{3-\delta}$ (BZY10) is evidenced by a well separated semicircle from impedance spectra with characteristic capacitance of ~$10^{-7}$ F.

The specific conductivities of grain boundaries and the Ag-BZY10 interface space charge layer were calculated on the basis of an ideal brick layer model and measured capacitances. Based on the Mott–Schottky approximation [5], the space charge layer potential, also known as the Schottky potential, was calculated for grain boundaries and the electrode interface vs temperature (300 – 550ºC), $pO_2$ ($10^{-5}$ – 0.98 atm) and $pH_2O$ (0.005 – 0.021 atm).

The Schottky potential at the electrode-electrolyte interface was found to be around 2 times higher than that of the grain boundaries, which for instance may arise from the segregation of protons at the interface in order to reduce the large lattice mismatch between the metal electrode and the perovskite oxide electrolyte. The potential increased with increasing $pH_2O$ for both grain boundaries and the Ag-BZY10 interface. The grain boundary potential decreased with increasing temperature, while $pO_2$ had little effect. For the Ag-BZY10 interface potential, there was an apparent interplay between the effects of temperature and $pO_2$. Interpretations of the above phenomena will be proposed and discussed.

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**Anjali Choubey-Poster**

Topic: Exploring near-earth nickelates as absorber material for tandem solar cell application

Abstract: Many classes of materials, are studied for photovoltaic applications. Gallium arsenide (GaAs) is highly efficient but expensive, silicon (Si) is well-established but approaching the theoretical limit, and halide-perovskites are developing rapidly but are toxic and unstable. Oxide-perovskites are non-toxic and remain stable during environmental, photobleaching, and thermal exposures. Additionally, they are well known and thoroughly studied for their electronic, magnetic, dielectric, superconducting, and catalytic properties, but not so much for photovoltaic properties. Hence, oxide-perovskites seem like an excellent candidate for investigation as an alternative to halide-perovskites for photovoltaic applications.

**Caitlin Micaela Guzzo**
NKS-FUM 2024
Poster presentation: Abstract

***Functional compositional engineering in lead-free piezoelectric bioceramics***

Caitlin Guzzo, Julia Glaum
Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Piezoelectric biomaterials have been investigated since the advent of lead-free piezoelectrics, with particular emphasis for use as orthopaedic implants. Human bone itself is piezoelectric, using electrical signals to guide bone repair and regrowth. A piezoelectric orthopaedic implant material could provide both the structural support of bone as well as the electrical signals necessary to stimulate endogenous bone growth. However, the performance of piezoelectric implant materials in biological conditions is not fully understood.

Herein we introduce a method for controlling compositional changes in sodium potassium niobate (KNN) to improve functional properties and reproducibility in solid- state processing. KNN-based ceramics were modified via stoichiometry and thermal processing environment. Following *in vitro* testing, characterisation involved electron microscopy, structural and chemical analysis, piezoelectric testing, and assessment of the effect of stoichiometry on local and bulk material structure.

Hygroscopic secondary phases (e.g. $K_4Nb_6O_{17}$) are often present in KNN due to local inhomogeneities, which arise from unequal diffusion rates and vapourisation of alkali species during processing. The presence of these hygroscopic phases leads to low stability in aqueous environments, and thus preclude the use of KNN as an orthopaedic implant. This work presents two approaches for reducing or eliminating these phases: (i) inducing a 2 mol% alkali excess, or (ii) by sintering stoichiometric KNN in a hybrid air- reducing atmosphere. Dimensional stability and electrical properties of these modified KNN materials were maintained over a 14-day *in vitro* study. 2 mol% alkali-excess KNN was shown to maintain significant piezoelectric properties while maintaining 24.4% open porosity. Pore and interconnect sizes were found to be larger than 10 µm, which is advantageous for tissue infiltration and osseointegration of bone tissue scaffolds. Stoichiometric KNN sintered in a hybrid atmosphere was found to maintain a piezoelectric coefficient of 89 pC/N after 14 days *in vitro*, with 11.7% open porosity. With both dimensional and electrical stability in simulated physiological environments, these KNN-based bioceramics are promising materials for orthopaedic implants.

# Advancing the Application Space of Barium Titanate ($BaTiO_3$) via ALD

D. Pulikkottil Dinesh, H. H. Sønsteby, O. Nilsen, M. Valldor

This project focuses on advancing low-temperature atomic layer deposition (ALD) for precise deposition of epitaxial barium titanate (BTO) thin films. By exploring controlled growth mechanisms and high temperature synthesis limitations, it aims to tailor BTO properties, including ferroelectric and photonic characteristics. The initial phase involves refining titanium dioxide ($TiO_2$) thin films using titanium tetra isopropoxide and ozone as precursors, aiming to elevate the ALD process and establish a robust foundation for subsequent BTO film deposition. In the subsequent stage, a stable barium precursor is introduced, offering an alternative pathway for BTO thin films via ALD.

The project's novelty extends to its commitment to extensive characterization, encompassing optical, chemical, structural, and electronic/electrical aspects. Advanced microscopy techniques will also be employed to provide a detailed understanding of the deposited films. This systematic optimization of the ALD process, coupled with thorough characterization, aims to achieve controlled and precise BTO thin film deposition at lower temperatures and for fine-tuning and improving their properties. The resulting insights are expected to contribute not only to the advancement of ALD technology but also to the expanded utilization of BTO in cutting-edge electronic and photonic devices, offering enhanced performance and customization.

# Minority bulk and surface proton conduction in ceramic positrodes for proton ceramic electrochemical cells

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## Abstract

The positrode is a critical component for proton ceramic steam electrolyzers and fuel cells for hydrogen and ammonia. It constitutes a major contribution to overpotentials and hense losses in the whole cell due to limited solubility and diffusivity of protons, which is challenging to characterise and improve for those predominantly electronic conductors. We are establishing theoretical frameworks and experimental methodology for measuring protonic conductivities on surfaces and in the bulk of positrode materials. According to our previous work on surface protonic conduction in porous oxides, we investigate the adsorption and dissociation of water on surfaces of electron conducting oxide electrode materials using nickel oxide (NiO), a p-type conductor as the model material.

**Acknowledgment:** This work is supported by **FME HYDROGENi** which is financed by its industry partners and the Norwegian government through the Research Council of Norway's Centres for Environment-friendly Energy Research programme (FMETEKN, project no. 333118)

# $Ba_{0.95}La_{0.05}(Fe_{0.7}Ni_{0.2}Zn_{0.1})O_{3-\delta}$ as steam electrode in proton ceramic electrochemical cells

**Stine Roen[1], Truls Norby[1], Ragnar Strandbakke[2] and Jonathan M. Polfus[1*]**

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Proton ceramic electrochemical cells (PCECs) convert electrical energy to and from hydrogen at intermediate temperatures (400-700 °C), but their efficiency is limited by the sluggish electrochemical reaction kinetics of the steam/air electrode (positrode), specifically the oxygen evolution reaction (OER) in proton ceramic electrolyzers (PCEs) and oxygen reduction reaction (ORR) in proton ceramic fuel cells (PCFCs).

Bulk protonic conduction may enhance positrode performance by increasing the electrochemically active area beyond the triple-phase boundaries. Significant hydration and proton conduction is observed in positrode perovskites like lanthanum doped barium ferrite (BLF) where the B-site is acceptor doped with Ni and Zn [1], [2]. To further explore the properties as a positrode, electrochemical impedance spectroscopy (EIS) are performed on $Ba_{0.95}La_{0.05}Fe_{1-x-y}Ni_xZn_yO_{3-\delta}$ (BLFNZ) deposited on proton conducting electrolyte $BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-\delta}$.

Various BLFNZ compositions are studied in a symmetrical cell with reference electrode. Key variables such as activation energies, pre-exponentials and predominant charge carriers are investigated by considering polarization resistance ($R_p$) as a function of $pO_2$ and $pH_2O$ across a wide temperature range. Extracting individual area specific polarization resistances ($R_{p,i}$) at open circuit voltage reflects equilibrium conditions, while applying cathodic and anodic DC voltage to EIS sweeps delineate ORR and OER conditions, respectively. The voltage application results in a net current ($I$) through the cell and $R_{p,i}$ is later converted into net overpotentials by integrating $R_{p,i}$ over $I$.

In this work combines EIS studies with thermogravimetric analysis (TGA) and isotope exchange to discern the electrochemical properties of $Ba_{0.95}La_{0.05}Fe_{0.7}Ni_{0.2}Zn_{0.1}O_{3-\delta}$ (BLFNZ10), amongst other BLFNZ compositions at temperatures 250-500 °C in varying $pO_2$ and $pH_2O$. Assuming hydration dominates the mass change in humid air, TGA experiments reveal that the proton concentration ranges from 1.8 mol% to 0.03 mol% for temperatures 250-500 °C, which remains at a significant level for bulk protonic conduction. However, BLFNZ10 appears to have a large activation energy, but a small pre-exponential value renders the $R_p$ comparable to state-of-the-art positrode materials [3]. The activation energy found by isotope exchange measurements suggest that it is a sluggish surface oxygen exchange reaction limiting the electrode reaction. Continued work on combining EIS data across various atmospheres and DC bias with TGA experiments yields further insight into the reaction mechanisms of BLFNZ10.

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# Modelling and characterization of negatrodes in proton ceramic electrochemical cells

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## Abstract

To address the ever-growing energy demand of modern society, promote the use of renewable energies and implement sustainable energy carriers like hydrogen, further technologies for the efficient energy conversion and storage are required. Proton Ceramic Electrochemical cells are a promising candidate to play a crucial role in those technologies. For the widespread application, certain challenges need to be overcome mainly concerning stability and efficiency of current cells due to e.g. the sluggish reaction kinetics of the steam/air electrode (positrode). To address this, in-depth studies of the reaction mechanisms are essential to understand the limitations of operating cells.

Therefore, we develop a finite element model of the two half-cell reactions aiming at the fundamental understanding of the electrodes and their limitations. Only fundamental kinetic parameters serve as input of the model based on theoretical and experimental studies such as DFT calculations and electrochemical measurements. The finite element model can be related to studies on microelectrodes with well-defined geometries which have been successfully employed to unravel different reaction pathways in solid oxide fuel cells. [1, 2]
The model electrodes are fabricated using common microstructuring techniques, i.e. photolithography and subsequent physical vapour deposition to form thin films.

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# Machine Learning-Guided Discovery of Laves Phases for Magnetocaloric Hydrogen Liquefaction

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**Three machine learning algorithms were used to predict the magnetic transition temperatures for light rare-earth-based Laves phase materials. PrCoNi and NdCoNi were selected as promising candidates for magnetocaloric hydrogen liquefaction, synthesized, and characterized. Synchrotron X-ray diffraction confirmed monophasic cubic (C15) Laves structures. Physical Property Measurement System measurements confirmed the magnetic transition temperatures to be in the relevant temperature range for magnetocaloric hydrogen liquefaction, in agreement with the machine learning predictions.**

Hydrogen liquefaction is important to make it a competitive energy carrier due to easier transportation because of increased energy density. Conventional hydrogen liquefaction is performed using a gas compression cycle, which has the drawback of a reduced efficiency at cryogenic temperatures. Therefore, magnetic cooling using the magnetocaloric effect (MCE) is a promising alternative [1]. The MCE involces heating and cooling of specific materials upon undergoing magnetization and demagnetization, respectively, quantified by the isothermal entropy change ($\Delta S_m$) and the adiabatic temperature change ($\Delta T_{ad}$) [1]. The largest MCE occurs at the magnetic transition temperature of the material, $T_c$. Therefore, materials with a $T_c$ between $20\,\mathrm{K}$ (the condensation temperature of hydrogen) and $77\,\mathrm{K}$ (the condensation temperature of nitrogen) can be relevant for hydrogen liquefaction. Many cubic (C15) Laves phase ($AB_2$) materials are possible candidates because of relevant $T_c$ [1].

Machine learning (ML) can be used to predict material properties given a sufficiently large database [2]. Random forest regression (RFR), gradient boosting regression (GBR), and neural networks (NNs) are ML methods that can successfully predict target features using a minimal number of descriptive features. In this work, these ML models predicted the $T_c$ of light rare-earth-based Laves compounds, using chemical composition as descriptors. PrCoNi and NdCoNi were chosen and synthesized using arc melting based on the predictions. The NdCoNi sample was annealed for 96 hours at $1073\,\mathrm{K}$, while the PrCoNi sample remained as-cast.

Uniform phase composition is important for magnetocaloric materials as secondary phases could exhibit magnetic transitions at different temperatures or no magnetic transitions, thus decreasing the $\Delta S_m$ and $\Delta T_{ad}$. Therefore, Synchrotron Radiation Powder X-Ray diffraction (SR-PXD) data were collected at station BM01 of the Swiss-Norwegian Beamlines (SNBL) at the ESRF (European Synchrotron Radiation Facility) in Grenoble, France. The measurements were performed at room temperature, using a beam with a wavelength of $0.7206\,\mathrm{\AA}$. The SR-PXD patterns showed that both samples have a cubic Laves phase and are monophasic.

Physical Property Measurement System (PPMS) measurements were performed to determine $T_c$ from the maximum of the derivative of the magnetization as a function of the temperature. The samples were cooled down to $5\,\mathrm{K}$ without an applied field, before a field of $2\,\mathrm{T}$ was applied for the PrCoNi sample and $1\,\mathrm{T}$ for the NdCoNi sample. Then heating and cooling were performed at a rate of $1\,\mathrm{K/min}$ without removing the applied field. Table I shows the predicted and experimentally determined $T_c$. The NN and GBR made the most precise predictions for PrCoNi and NdCoNi, respectively. The $T_c$ values predicted by the three ML models differed by up to $27\,\mathrm{K}$ from the experimental ones. The RFR model had a test mean absolute error (MAE) of $25\,\mathrm{K}$, the GBR model had an MAE of $20\,\mathrm{K}$, while the NN model had an MAE of $30\,\mathrm{K}$, explaining the error of the predictions. This discrepancy is likely due to the low number of light rare-earth-based cubic Laves phases in the literature used to build the database. Despite this difference between predicted and experimental $T_c$, the experimental $T_c$ values were still in the relevant temperature range for magnetocaloric hydrogen liquefaction. The difference between the predictions made by each model is attributed to the three models making predictions in different ways which could lead to different conclusions.

TABLE I
THE $T_c$ PREDICTED BY RFR, GBR, NN, AND THE EXPERIMENTAL $T_c$ DETERMINED FROM THE MAXIMUM DERIVATIVE OF THE MAGNETIZATION AS A FUNCTION OF TEMPERATURE USING PPMS DATA.

| Compound | $T_c$ RFR (K) | $T_c$ GBR (K) | $T_c$ NN (K) | $T_c$ exp. (K) |
|---|---|---|---|---|
| PrCoNi | 49 | -2 | 20 | 23 |
| NdCoNi | 63 | 25 | 51 | 36 |

Magnetic hysteresis curves were measured at $10\,\mathrm{K}$ with a magnetic field sweep rate of $0.2\,\mathrm{K/min}$ to find the saturation magnetization of the samples. According to the measurements, PrCoNi exhibited a saturation magnetization of $42\,\mathrm{emu/g}$ while NdCoNi had $32\,\mathrm{emu/g}$ at a field of $2\,\mathrm{T}$.

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# Performance and degradation of positrodes for proton ceramic electrolysers

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## Abstract

Proton ceramic electrolysers (PCEs) that utilise available steam and/or heat (renewable or industrial) as a supplementary energy source provide superior electrical efficiency compared to conventional water electrolysis. The positrode constitutes a major contribution to the overpotentials and hence losses of PCEs, resulting from its low solubility of protons, as well as limiting surface kinetics of the oxygen evolution reaction (OER) – which are challenging to characterize and improve.

The positrode needs to use its surface for the redox reaction between water vapour, electrons, and protons and to form oxygen. The protons are supplied from the electrolyte via diffusion in the positrode bulk and surfaces. The rate of the surface reaction and the proton charge transfer reaction at the 2pb as well as the ratio between the diffusivity of protons in the bulk and on the surface will determine how far the protons go on the surface before diving into the bulk. The sole transport on the surface to charge transfer only at the 3pb must be considered a limiting case. The microstructure of the positrode and its surface and interface to the electrolyte is key to efficient heterogeneous reaction kinetics and transport of electrons and protons as well as long-term stability.

In our ongoing research, we aim to establish theoretical frameworks and experimental methodology to measure and interpret the parameters that determine the kinetics and transport overpotentials and to evaluate which ones limit performance and cause degradation. The measured parameters are input to finite element modelling necessary to handle the complexity of processes and geometries. We report impedance spectroscopy and voltammetry for 3-electrode setups for selected positrode materials as a function of temperature and oxygen and steam partial pressures and extract parameters along geometrical and mechanistic models. The results are interpreted in terms of ohmic, charge transfer, and mass transfer (combined diffusional and surface kinetic Gerischer-type) polarisation. We also follow parameters over time to elucidate degradation mechanisms. The results will serve as input for finite element modelling, to evolve the mechanistic electrochemical model, improving the performance of operating cells, and counteracting degradation.

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*Effect of ionic shape and size in dictating piezoelectric property of organic plastic ionic crystals*

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Ferroelectric materials have been used as the temperature and pressure sensor for their inherent pyroelectric and piezoelectric properties. Organic ferroelectric materials hold tremendous potential in this respect owing to their flexibility, solution processability, and light-weight nature leading to easy fabrication over large surface area. However, the organic ferroelectrics lack many advanced properties of conventional metal oxide ferroelectrics including high Curie temperature, large values of piezoelectric coefficient, and multi-axial polarization on applied electric field or pressure. To witness the advanced properties in molecular ferroelectric materials, the 'plastic ionic crystals' (PICs) have been explored as the sustainable room temperature ferroelectrics. Plastic ionic crystals (PICs) are comprised of spherical ions, and exhibit a room temperature plastic *meso*-phase in which the ions show long range positional order but short range rotational disorder. Organic inorganic hybrid materials have attracted wide attention as the PICs with Curie temperature ($T_c$) above the room temperature, and piezoelectric coefficient comparable to the inorganic oxide ferroelectrics.

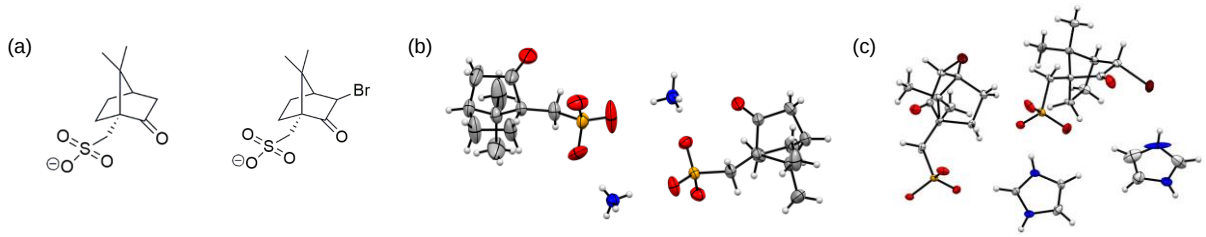


Fig 1. (a) Quasi-spherical anions used for the study, (b) Crystal structure of **1**, (b) Crystal structure of **2**.

Pure 'organic' PICs surpass the hybrid PIC materials in terms of flexibility and sustainability, however, their number is limited due to the proper choice of the constituent ions. The use of 'homochiral' substituents have been considered as an effective strategy to ensure room temperature ferroelectricity in pure organic PICs. In this work, we report two pure organic plastic ionic crystals: (a) ammonium salt of (1S)-10-camphorsulphonate (**1**), (b) imidazolium salt of (1S)-3-bromo-10-camphorsulphonate (**2**). The systems **1** and **2** crystallize in chiral-polar $C_2$ and chiral $P2_12_12_1$ space group respectively at room temperature. In these systems, the chiral and quasi-spherical (1S)-10-camphorsulphonate (or mono-brominated derivative) anion were used, while the cations were varied between the spherical ammonium to planar, aromatic imidazolium to witness the role of size and shape of ions in dictating the piezoelectric property.

# Electrodics for proton ceramic electrochemical cells

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The impact of efficient solid-state electrochemical energy conversion requires improved electrolytes for protons, oxide ions, or alkali metal ions, but also energy- and cost-efficient electrodes. State-of-the-art electrodes depend on mixed electronic and mass transport as well as electrocatalytic activity and optimized microstructures. The entangled materials chemistry and electrochemistry along with 2- or 3-phase microstructures makes electrode processes challenging to describe and model from fundamental microscopic to effective medium macroscopic levels. This is a goal of the collaboration in several ongoing projects on proton ceramic electrochemical cells between University of Oslo, SINTEF Industry, CoorsTek Membrane Sciences AS, and European partners, in which we combine DFT and finite element modelling with a range of characterization techniques to identify rate-limiting steps and degradation processes in order to systematically improve electrode performance and lifetime.

The polarization processes at solid-state electrodes comprise space charge layer depletion resistance, charge transfer between the electrolyte and electrode phases, and mass transfer in and on the electrode material. The latter comprises diffusion in and on the solid electrode material and in the gas phase as well as surface reaction kinetics. The processes on Ni metal negatrodes involves diffusion of dissociated atomic hydrogen, [1] while the processes on mixed proton-electron conducting oxide positrodes involves proton-proton charge transfer, proton diffusion, and surface electron transfer oxygen-steam redox-reaction.

Electrochemical impedance spectroscopy (EIS) enables separation of the different polarisation processes by their capacitances ranging over more than 12 orders of magnitude. The mass transfer is interpreted in terms of Gerischer impedances that describe coupled diffusion and reaction kinetics control as well as the chemical capacitance of porous mixed conducting electrodes. Individual polarisation resistances measured by EIS under DC bias can be integrated over current to obtain individual overpotential-current curves and help to identify processes and predicting behaviours under operation in fuel cell or electrolyser mode.[2]

Parallels to polarisation impedances of other solid-state devices such as oxide ion conducting solid oxide electrochemical cells and solid-state Li ion batteries will be drawn where possible.

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# Charge and mass transfer polarisation of BGLC37 positrodes for proton ceramic electrochemical cells

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## Abstract

Double perovskite oxide $BaGd_{0.3}La_{0.7}Co_2O_{6-\delta}$ (BGLC37) is known as one of the best positrodes for proton ceramic electrochemical cells. In this work, the effect of electrode sintering temperature (925 vs 1150°C) and electrode-electrolyte interface microstructure (with and without an electrode functional layer, FL) on the electrochemical performance of BGLC37 positrode on $BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-\delta}$ (BZCY721) electrolyte were investigated under wet air conditions ($pH_2O$ = 0.025 atm) using impedance spectroscopy. Improved interfacial microstructure contributed to reducing both ohmic and polarization resistances. Additionally, a lower electrode sintering temperature resulted in a decrease in ohmic resistance. On the other hand, a higher sintering temperature proved more effective for lowering electrode polarization resistance, exhibiting activation enthalpies of approximately 1.7 eV above 600°C and 1.3 eV below 600°C, as shown in Figure 1c. Notably, we also observed distinct dependencies on the atmosphere (wet vs dry) concerning both ohmic and polarization resistances.

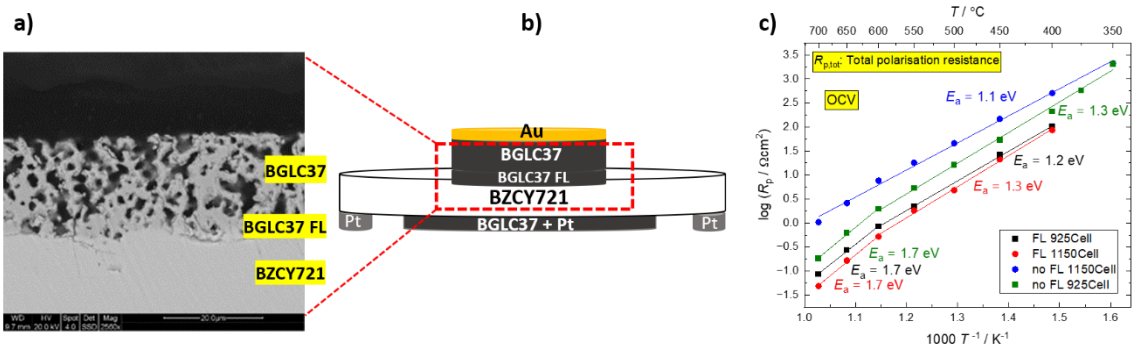


**Figure 1** a) SEM cross-section micrograph showing the top BGLC37 electrode on BZCY721 electrolyte, b) the three-electrode setup for electrochemical characterization, c) the effect of the electrode sintering temperature and the interfacial microstructure on the total polarization resistance of BGLC37 in wet air ($pH_2O$ = 0.025 atm).

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