

Programme & Abstracts

OPERA Workshop — General Workshop (second part)

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30 September – 2 October 2026

La Cristalera, Carretera M-611 km 10
28792 Miraflores de la Sierra, Madrid

Chair: Celia Polop (UAM)
Scientific committee: Qiong Cai (Surrey) · Peter Siffalovic (CEMEA SAS)

Funded by the European Union

OPERA Project (Horizon EU) · horizon-opera.eu/final-opera-workshop-in-madrid

OPERA Workshop — Programme Overview

General Workshop, 30 September – 2 October 2026

La Cristalera, Miraflores de la Sierra, Madrid



La Cristalera, Miraflores de la Sierra (Madrid) — workshop venue

Wednesday 30 Sep

09:00 *Welcome & opening*

IMAGING & MICROSCOPY

09:15 **Juan de la Figuera**
09:55 **Till Fuchs**
10:35 Michael Foerster
11:00 *Coffee break*

X-RAY IMAGING & DIFFRACTION

11:30 **Chun Ann Huang**
12:10 **Santhana Eswara Moorthy**
12:50 François Liénard
13:15 *Lunch*

OPERANDO SPECTROSCOPIC PROBES

14:45 **Rosalía Cid Barreno**
15:25 **Juan Miguel López del Amo**
16:05 **Ashley Black**
17:00 *Coffee break & poster*
19:00 *Dinner*

Thursday 1 Oct

OPERANDO ELECTROCHEMICAL & DIFFRACTION METHODS

09:00 **Maria Alfredsson**
09:40 **Jake Huang**
10:20 Peter Siffalovic
10:45 *Coffee break*

SOLID ELECTROLYTE MATERIALS I

11:15 **Venkataraman Thangadurai**
11:55 Kristian Nikolowski
13:00 *Lunch*

SOLID ELECTROLYTE MATERIALS II

14:15 **Carolina Rosero-Navarro**
14:55 Enrique Vasco Matias
15:20 *Prep. & coach boarding*
16:00 **Departure for Segovia**

Friday 2 Oct

BEAM-BASED CHARACTERIZATION & MULTISCALE MODELLING

09:00 **Benedetto Bozzini**
09:40 **Gastón García López**
10:20 Qiong Cai
10:45 *Closing remarks*



Programme - General Workshop (second part)

Chair: Celia Polop (UAM) · Scientific committee: Qiong Cai (Surrey), Peter Siffalovic (SAS)

Invited talks 40 minutes (30 + 10 questions), shaded. Contributed talks 25 minutes (20 + 5 questions). Every session opens with an invited talk.

Wednesday 30 September 2026

Day 1 - full day

09:00 **09:15**	15 min	**Welcome and opening of the General Workshop** Chair / Scientific Committee	
SESSION 1 - Imaging & microscopy			Chair: Celia Polop
09:15 **09:55**	Invited 40 min	**Juan de la Figuera** Instituto de Química Física Blas Cabrera CSIC	Seeing oxides grow in low-energy electron microscopy: from ferrites to tungstates
09:55 **10:35**	Invited 40 min	**Till Fuchs** Justus Liebig University Giessen	Microstructure and Chemistry at Work: Operando EBSD and ToF-SIMS of Interfaces in Solid-State Batteries
10:35 **11:00**	Contributed 25 min	**Michael Foerster** ALBA Synchrotron	Early stage of anode formation investigated by VE-LEEM and synchrotron spectromicroscopy
11:00 **11:30**	30 min	**Coffee break**	
SESSION 2 - X-ray imaging & diffraction			Chair: Qiong Cai
11:30 **12:10**	Invited 40 min	**Chun Ann Huang** Imperial College London	Operando X-ray imaging and processing of structures inside lithium batteries
12:10 **12:50**	Invited 40 min	**Santhana Eswara Moorthy** Luxembourg Institute of Science and Technology	OPINCHARGE project - Selected highlights and broader perspectives
12:50 **13:15**	Contributed 25 min	**François Liénard** ID13, European Synchrotron Radiation Facility (ESRF)	Probing spatial heterogeneities in batteries with nano/micro X-ray diffraction
13:15 **14:45**	90 min	**Lunch**	
SESSION 3 - Operando spectroscopic probes			Chair: Peter Siffalovic
14:45 **15:25**	Invited 40 min	**Rosalía Cid Barreno** CIC energiGUNE	Operando Insights into Interphase Dynamics at Metal–Electrolyte Interfaces
15:25 **16:05**	Invited 40 min	**Juan Miguel López del Amo** CIC energiGUNE	Probing battery interfaces and electrochemical processes by ex situ and operando solid-state NMR
16:05 **16:45**	Invited 40 min	**Ashley Black** Instituo de Ciencia de Materiales de Barcelona CSIC	Probing Battery Reaction Mechanisms Operando: From Synchrotron Infrared and X-ray Spectroscopy to Beam-Induced Effects
17:00 **18:30**	90 min	**Coffee break & poster session** Open discussion	
19:00 **21:00**	120 min	**Dinner**	

Thursday 1 October 2026

Day 2 - full day

SESSION 4 - Operando electrochemical & diffraction methods			Chair: Kristian Nikolowski
09:00 **09:40**	Invited 40 min	**Maria Alfredsson** University of Kent	A Case Study on NMC622: Developing a Multimodal Operando Metrology and Modelling Framework for Mechanistic Insights
09:40 **10:20**	Invited 40 min	**Jake Huang** University of Muenster	Accelerated, Interpretable Operando Impedance Characterization for Solid-State Batteries
10:20 **10:45**	Contributed 25 min	**Peter Siffalovic** Centre for Advanced Materials Application SAS	Operando XRD: From synchrotron to laboratory
10:45 **11:15**	30 min	**Coffee break**	
SESSION 5 - Solid electrolyte materials I			Chair: François Liénard
11:15 **11:55**	Invited 40 min	**VenkataramanThangadurai** University St-Andrews	Garnet-Based Solid-State Li Metal Batteries
11:55 **12:20**	Contributed 25 min	**Kristian Nikolowski** Fraunhofer IKTS	Sulfide solid electrolytes: kinetic limitations in composite cathodes and the path towards commercialization
13:00 **14:15**	75 min	**Lunch**	
SESSION 6 - Solid electrolyte materials II			Chair: Michael Foerster
14:15 **14:55**	Invited 40 min	**Carolina Rosero-Navarro** Instituto de Ceramica y Vidrio CSIC	Glass and Glass-Ceramic Composite Electrolytes for Enhanced and Stable Interfaces with Lithium Metal
14:55 **15:20**	Contributed 25 min	**Enrique Vasco Matias** Instituo de Ciencia de Materiales de Madrid CSIC	Progress in Electrodes for Thin-Film Batteries
15:20 **16:00**	40 min	**Preparation and coach boarding for Segovia**	
16:00	**SOCIAL PROGRAMME - departure for Segovia** Guided visit of the city of Segovia, followed by dinner there. Return to La Cristalera in the evening.		

Friday 2 October 2026

Day 3 - half day

SESSION 7 - Beam-based characterization & multiscale modelling			Chair: Enrique Vasco Matias
09:00 **09:40**	Invited 40 min	**Benedetto Bozzini** Politecnico di Milano	Zn-air batteries investigated with complementary spectroscopy and imaging approaches
09:40 **10:20**	Invited 40 min	**Gastón García López** Autonomous University of Madrid	Ion beam analysis: a tool for battery research and beyond
10:20 **10:45**	Contributed 25 min	**Qiong Cai** University of Surrey	AI assisted multiscale modelling of metal anode-electrolyte interfaces in solid state batteries
10:45 **11:00**	15 min	**Closing remarks** Chair / Scientific Committee	

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OPERA Workshop
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Seeing oxides grow in low-energy electron microscopy: from ferrites to tungstates

Juan de la Figuera[1]

[1]*Instituto de Química Física Blas Cabrera, Dpto. Química Física de Materiales, Madrid, Spain*

Corresponding author: juan.delafiguera@csic.es

High-quality growth of materials is an underlying requirement in material science. And one of the reference growth methods in for high-quality nanostructures is molecular beam epitaxy (MBE). However, oxide growth by MBE has complications: often different phases are possible, and the morphology can be very different from a simple flat continuous layer. Thus there is the need to study their growth by techniques that allow the real-time observation of the growth front during growth, and the structural and chemical characterization of nanometer sized areas of the films once grown. In this work we will describe how we use low-energy electron microscopy to investigate in real time the growth of oxide nanostructures on metals by high-temperature oxygen-assisted molecular beam epitaxy. To characterize them we resort to selected area low-energy electron diffraction and x-ray spectroscopies, combining it with photoemission microscopy as well as ex-situ atomic force microscopy and Raman spectroscopies. We will show what surprises await us when we explore different substrates.

This work was supported by the laboratorio de caracterización "Ramón Gancedo", REDLAB-023, https://labrg.iqf.csic.es



Microstructure and Chemistry at Work: Operando EBSD and ToF-SIMS of Interfaces in Solid-State Batteries

Till Fuchs[1]

[1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany.

Solid-state batteries are studied so intensively because a non-flammable solid electrolyte may finally allow the use of a lithium metal anode. Lithium metal combines a low redox potential of −3.04 V with a high specific capacity of 3861 mAh g^{-1}, promising an improved energy density. The concept can be pushed even further in metal reservoir free ("anode-free") cells, in which the lithium is plated *in situ* at a current collector during the first charge. This removes excess metal, simplifies cell fabrication and avoids the handling of reactive lithium foils, but it also makes the cell performance fully dependent on how uniformly the metal is deposited and dissolved.

Since plating and stripping constantly reshape the metal layer, methods that follow the morphology while the cell is running are extremely valuable. Operando scanning electron microscopy at Cu|LLZO model-interfaces showed that the lithium growth mode depends strongly on the applied current density, with higher current densities leading to a higher particle density.[1] Beyond pure imaging, electron backscatter diffraction (EBSD) adds crystallographic information. A dedicated preparation and operando measurement makes the grain structure of electrodeposited lithium and sodium accessible and reveals columnar grains larger than 100 µm, a preferential orientation of grain boundaries, dynamic grain coarsening during deposition and pore formation within grains during dissolution.[2]

Electron microscopy and diffraction, however, deliver only limited chemical information, which is exactly what is needed to understand interphase formation and side reactions. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) closes this gap, as it detects all elements including lithium with high surface sensitivity and provides chemical images in 2D and 3D. Exemplarily, in situ ToF-SIMS on lithium|solid electrolyte interfaces was used to classify the stability of different solid electrolytes and to identify a Li^2S rich interlayer of roughly 250 nm at the Li|Li^6PS^5Cl interface.[3] With a purpose-built operando sample holder, full cells can now be cycled inside the instrument. This allowed us to follow the iodide/iodine redox mediation in LiI containing lithium sulfur composite cathodes directly during charging, where the I^{2-} signal rises steeply once the oxidation potential of I^- is reached.[4]

Combining these operando methods connects morphology, microstructure and chemistry, and thereby provides the mechanistic understanding needed for stable solid-state batteries.

References

[1] T. Fuchs & J. Becker et al. Current-Dependent Lithium Metal Growth Modes in "Anode-Free" Solid-State Batteries at the Cu|LLZO Interface. *Adv. Energy Mater*., 13, 2203174 (**2023**).

[2] T. Fuchs et al. Imaging the microstructure of lithium and sodium metal in anode-free solid-state batteries using electron backscatter diffraction. *Nat. Mater*. 23, 1678–1685 (**2024**).

[3] S.-K. Otto et al. In Situ Investigation of Lithium Metal–Solid Electrolyte Anode Interfaces with ToF-SIMS. *Adv. Mater. Interfaces*, 9, 2102387 (**2022**).

[4] T. Weintraut et al., submitted to *ACS Energy Letters* (**2026**).

Early stage of anode formation investigated by VE-LEEM and synchrotron spectromicroscopy

J. Díaz-Sánchez[1,2], P. Hernández-Martín[1,2], N. Kwiatek-Maroszek[3], H.R. Bratlie[4], R. Anton[5], A. Lowack[5], A. Galindo[6], K. Kataoka[7], E. Vasco[6], K. Nikolowski[5], D. Rettenwander[4], E.G. Michel[1,2,8], M.A. Niño[3], M. Foerster[3], C. Polop[1,2,8]

[1]Condensed Matter Physics Department, Autonomous University of Madrid (UAM), Spain
[2]Nicolás Cabrera University Institute of Materials Science (INC), UAM, Spain
[3]ALBA Synchrotron Light Facility, Cerdanyola del Vallès, Spain
[4]Norwegian University of Science and Technology (NTNU), Trondheim, Norway
[5]Fraunhofer Institute for Ceramic Technologies and Systems (IKTS), Dresden, Germany
[6]Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas (CSIC), Spain
[7]National Institute of Advanced Industrial Science and Technology (AIST), Research Institute for Energy Efficient Technologies, Japan
[8]Condensed Matter Physics Center (IFIMAC), UAM, Spain

Within OPERA, the Virtual Electrode LEEM (VE-LEEM) platform has been developed as multimodal surface microscopy approach to study with high resolution otherwise hard to access battery interfaces. Using the electron gun of the Low Energy Electron Microscope (LEEM), we grow in-situ alkali metal anodes (Li, Na) on solid state electrolytes (SSE) without any physical current collector and with precise control of the interaction energy (0-15 eV). Different early stage anodes are characterized by a combination of LEEM, UV and x-ray PhotoEmission Electron Microscopy (PEEM) and AFM; elucidating details of their growth mode and an asymmetric discharging path under positive charge from photoemission. These results can be understood to arise from the surface energies, exhibiting similar mechanisms as in conventional thin film growth studies [1].

In this talk we will give a summary of our findings on the early stage anode growth and stripping in the Li/LLZTO and Na/NaGdSiO systems. We will also present ongoing research on the integration of metallic interlayers and their effect on the anode microstructure and report on the progress of ongoing work addressing the interface between anode and SSE.

References

[1] *J. Díaz-Sánchez et al., Nanoscale imaging reveals critical plating and stripping mechanisms in anode-free lithium and sodium solid-state batteries, arXiv:2603.00998 (2026).*

Operando X-ray imaging and processing of structures inside lithium batteries

Chun Huang[1], *Chu Lun Alex Leung*[2], *Matthew D. Wilson*[3]

[1]*Department of Materials, Imperial College London, London, SW7 2AZ, UK*

[2]*Department of Mechanical Engineering, University College London, London, WC1E 7JE, UK*

[3]*STFC-UKRI, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK*

Corresponding author: *a.huang@imperial.ac.uk*

It is conventionally difficult to measure lithium ion concentrations inside commercially standard battery cell configurations using X-rays because the weak signals of lithium cannot be distinguished from the strong signals of other heavy transition metal elements that are present in batteries. Here, we show a novel *operando* imaging technique of X-ray Compton scattering imaging that maps lithium ion concentration distributions and then use X-ray computed tomography (XCT) to show 3D electrode microstructural changes and lithium dendrite growth inside batteries during charging and discharging [1,2]. The results are complemented by time-of-flight secondary ion mass spectrometry (ToF-SIMS) and cryo-plasma focused ion beam (cryo-PFIB) to study effects of pressure inside zero-excess lithium batteries on lithium chemical distributions and physical structures [3].

Using the insights uncovered by characterisation, we develop two advanced processing methods to make electrode microstructure that speeds up lithium ion diffusion, one is directional ice templating for making electrodes with vertical pores for lithium ion batteries with liquid electrolyte, and the other is directional freezing and polymerisation for fabricating cathodes with vertical columns of cathode material and solid polymer electrolyte for solid-state lithium metal batteries. The method directly incorporates the solid polymer electrolyte in the electrode structure within a single process.

References

[1] C. Huang, M.D. Wilson, et al., Advanced Science, 9 (2022) 2105723.

[2] C. Huang, M.D. Wilson, et al., Journal of Physics: Energy, 7 (2025) 025009.

[3] J. Su, C. Huang, Energy & Environmental Science, 18 (2025) 8815.

OPINCHARGE project - Selected highlights and broader perspectives

Santhana Eswara[1], Sayantan Sharma[1]

[1]*Advanced Instrumentation for Nano-Analytics (AINA) Luxembourg Institute of Science and Technology 41, rue du Brill, L-4422 Belvaux, Luxembourg*

Corresponding author: *santhana.eswara@list.lu*

This presentation will review a selection of key highlights and achievements of the OPINCHARGE project. Specific emphasis will be on the advances of operando imaging using Secondary Ion Mass Spectrometry (SIMS). We will discuss proof-of-concept demonstrations of operando microscopy which enable correlative analysis of microstructural, chemical and electrochemical evolution of battery materials [1]. With the use of isotopic labeling, we captured the localized spatial variations of Li^+ distribution during constant-current charging across a gel polymer electrolyte. Furthermore, the role of the substrate material (Cu) and interlayers (Au or Ag) in governing the lithium plating characteristics for anode-free batteries was investigated using isotope labeling. On bare Cu substrate, ex-situ isotope-selective imaging confirmed inhomogeneous Li plating and time-dependent variations in Li^+ flux distributions. On the contrary, with an interlayer of Au or Ag, the Li plating was confirmed to be more homogeneous, which is desirable to prevent Li dendrite formation [2]. The isotope labeling experiments were complemented by operando imaging using neutrons which was performed in cooperation with the project partner Paul Scherrer Institute in Switzerland.

An important limitation in general for charged particles (or photons)-based analytical methods is radiation damage. To address this, we developed advanced raster scanning protocols for microscopy using ion and electron-beam. Together with the project partner German Research Center for Artificial Intelligence (DFKI), low-dose and high-speed image acquisition modes were developed wherein an initial acquisition of a random sparse image is analyzed “on the fly” to determine the subset of pixels to be probed in the next iteration of image acquisition. This opens the door to low dose as well as high-speed image acquisition. We will briefly discuss the imaging protocols and the trade-offs between lateral resolution, dose and time resolution.

Finally, we will present an example of a broader impact for the operando/in-situ SIMS imaging methodology. Specifically, a special SIMS sample holder was developed to perform simultaneous microscopy, chemical imaging and in-situ electrochemistry experiments for applications beyond battery research [3]. The results from these studies will also be briefly presented.

References

[1] S. Sharma et al, Electrochimica Acta 536 (2025) 146728

[2] S. Sharma et al, ACS Applied Materials & Interfaces (2026), accepted, DOI: 10.1021/acsami.6c06240

[3] A. Suresh Kumar, International Journal of Hydrogen Energy 214 (2026) 153705

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Probing spatial heterogeneities in batteries with nano/micro X-ray diffraction

François Liénard[1], Manfred Burghammer[1], Henrik R. Bratlie[2], Verena Reisecker[2], Juraj Todt[3], Pablo Hernandez Martin[4], Tobias M. Huber[5], Celia Polop[4], Jozef Keckes[3], Daniel Rettenwander[2].

[1]ID13, European Synchrotron Radiation Facility (ESRF), Grenoble, France
[2]NTNU, Trondheim, Norway
[3]Montanuniversität Leoben, Austria
[4]UAM, Madrid, Spain
[5]Huber Scientific, Vienna, Austria

Corresponding author: francois.lienard@esrf.fr

Batteries are inherently complex due to the electro-chemical and mechanical phenomena happening either at their interfaces or in their bulk[1,2]. Whether liquid or solid, batteries involve several critical phenomena that govern their operation. Accessing the spatio-temporal distributions of physical variables such as the phase, the microstructure or the stress can help to disentangle the interplay of these phenomena. For that matter the ID13 beamline has been more and more often used for battery experiments this past decade. In this presentation, we will present a general view of the state-of-the art at ID13[3], also covering recent Opera R&D results, before focusing on post-Opera opportunities for the community interested in employing X-ray micro-/nano-beam scanning diffraction methods. In the context of ongoing refurbishment activities at ID13 we will discuss possible experimental modes for solid-state battery research such as expanding the energy range, enabling multi-scale experiments, 3D-methods, and sub-millisecond time resolution. This should help spawning further discussions on related future requirements and how they can be met.

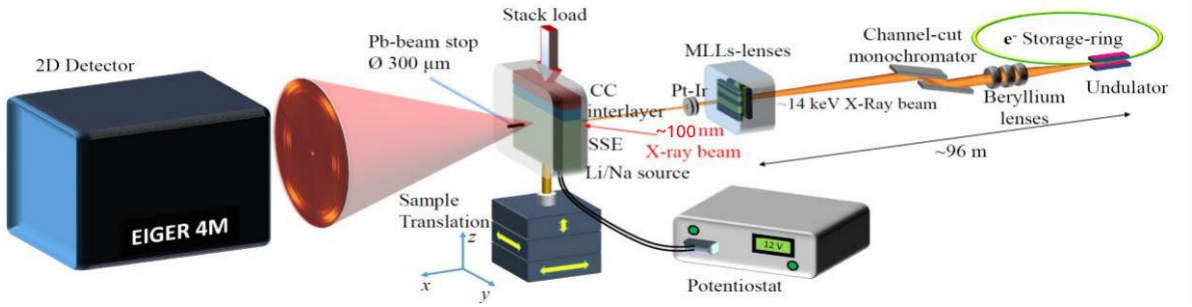


Figure 1. General overview of the ID13 setup applied to a battery for micro-/nano-beam scanning diffraction.

References

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*[3] Jacquet, Q., Cele, J., Casiez, L. et al. Operando microimaging of crystal structure and orientation in all components of all-solid state-batteries. Nat Commun **16**, 11524 (2025). https://doi.org/10.1038/s41467-025-66306-6*



Operando Insights into Interphase Dynamics at Metal–Electrolyte Interfaces

Rosalía Cid[1]

[1]*CIC energiGUNE, Basque Research and Technology Alliance (BRTA), 01510 Vitoria-Gasteiz, Spain*

rcid@cicenergigune.com

Metal–electrolyte interfaces critically influence the efficiency, stability and lifetime of next-generation metal batteries. However, their buried, highly reactive and continuously evolving nature makes it difficult to directly relate interfacial chemistry and metal transport to electrochemical performance.

In this contribution, operando X-ray photoelectron spectroscopy (OpXPS), combined with electrochemical and electron microscopy methods, is used to investigate the formation and evolution of metal–electrolyte interphases in lithium-based solid-state batteries. A virtual-electrode OpXPS approach induces Li migration and deposition directly within the XPS analysis area, providing time-resolved access to the earliest stages of interphase formation without exposing a buried interface ex situ.

For the halide solid electrolyte $Li_3YCl_4Br_2$ (LYCB), operando measurements show that the Li|LYCB interphase does not evolve as a static, homogeneous decomposition layer. Instead, Li plating drives chemical and spatial redistribution of reaction products, progressively generating a stratified interphase. Complementary impedance spectroscopy further indicate that electrochemical operation influences interfacial contact and transport as well as interphase chemistry.

The methodology is also applied to the garnet electrolyte $Li_7La_3Zr_2O_{12}$ (LLZO), with and without sputtered Cu thin-film current collectors. These experiments provide insight into Li transport through ultrathin Cu films and the subsequent accumulation of Li beneath the collector, linking nanoscale transport processes with the deformation and fracture observed in cycled anode-free Cu|LLZO cells.

Finally, current-collector engineering is extended to anode-free sodium systems, where metallic and alloy-forming interlayers modify nucleation, metal–collector interactions and deposition morphology.

Together, these studies show how operando surface analysis can connect interfacial chemistry, metal transport and mechanical evolution, providing mechanistic guidelines for designing more stable Li- and Na-metal battery interfaces

References

*[1] P. Lannelongue et al., Energy Storage Materials **72** (2024) 103733.*

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Probing battery interfaces and electrochemical processes by ex situ and operando solid-state NMR

Juan Miguel López del Amo[1]

[1] *Centre for Cooperative Research on Alternative Energies (CIC energiGUNE), Basque Research and Technology Alliance (BRTA), Vitoria-Gasteiz, Spain*

Corresponding author: *jmlopez@cicenergigune.com*

Next-generation batteries increasingly rely on solid electrolytes, lithium-metal anodes and high-capacity silicon-based electrodes, but their performance is often governed by buried interfaces and interphases that are difficult to access directly. Understanding these regions requires identifying the phases that form, determining whether ions can cross them, and establishing how they evolve during electrochemical operation.

Solid-state nuclear magnetic resonance (NMR) provides element-selective information linking interfacial composition and structure to ionic dynamics and electrochemical function. Here, ex situ and operando NMR are combined across several battery architectures to illustrate how these complementary approaches can resolve buried-interface chemistry and evolution during cycling.

In ceramic–polymer composite electrolytes, exchange NMR reveals lithium communication between inorganic and polymeric phases and shows how ceramic surface chemistry controls interfacial transport.[1] Studies of polymer–sulfide and sulfide–halide combinations identify spontaneous reaction products and establish how interphase formation affects lithium mobility and functional compatibility.[2,3] At lithium-metal interfaces, solid-state NMR shows that reduction of a halide electrolyte can generate a chemically stratified interphase compatible with reversible lithium plating and stripping.[4] In silicon–graphite composite anodes, ex situ NMR further reveals how electrolyte formulation controls the composition, organization and dynamics of the solid-electrolyte interphase (SEI), as well as its relationship with lithiated active materials.[5]

Operando measurements extend this picture by continuously cycling cells inside the NMR probe while spectra are acquired without interrupting operation. In gel-polymer and inorganic solid-electrolyte cells, lithium redistribution, interphase evolution and plating/stripping processes can be followed directly. Operando measurements on silicon–graphite electrodes track the reversible evolution of lithium environments during lithiation and delithiation, while changes in the metallic-lithium resonance provide information on the accumulation and morphological evolution of deposited lithium. Recent developments in operando cell design, including coin-cell geometries, further expand the electrochemical configurations accessible to NMR.

Together, these results show how ex situ NMR identifies interphases and probes ion transport, whereas operando NMR reveals when and how electrochemical processes develop under working conditions.

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[1] P. Ranque et al., J. Mater. Chem. A 9 (2021) 17812–17820.

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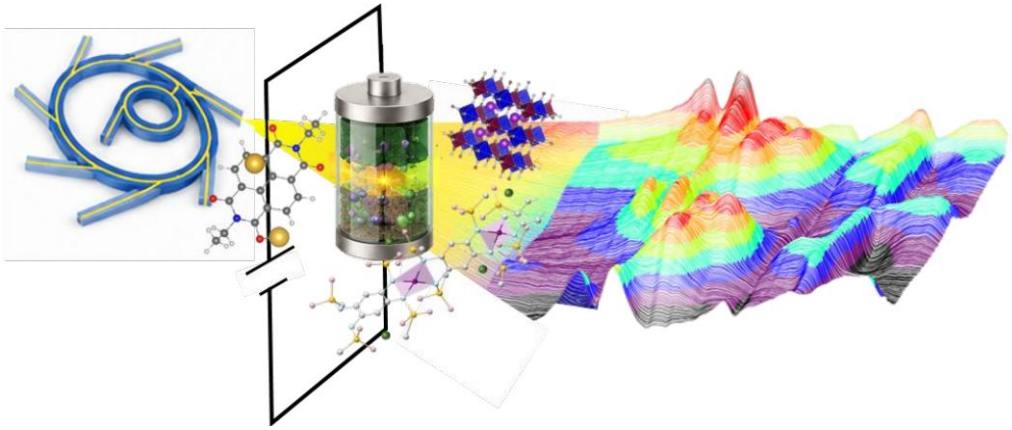
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Probing Battery Reaction Mechanisms *Operando*: From Synchrotron Infrared and X-ray Spectroscopy to Beam-Induced Effects

Ashley P. Black[1] on behalf of collaborators

[1] *Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Catalonia, Spain.*



Understanding electrochemical reaction mechanisms under realistic operating conditions remains a major challenge for the development of next-generation energy storage technologies. *Operando* synchrotron-based characterization techniques provide unique opportunities to probe structural and chemical evolution in real time, offering simultaneous temporal and spatial resolution inaccessible to conventional ex situ approaches. In this contribution, we present several case studies illustrating how *operando* synchrotron methodologies can elucidate reaction mechanisms across advanced battery chemistries. First, we demonstrate the capabilities of operando synchrotron-based Fourier transform infrared microspectroscopy (SR-μFTIR), exploiting sub-second acquisition times and micrometric spatial resolution to monitor dynamic electrochemical transformations in polyimide-type organic polymer electrodes.[1] We then apply operando SR-FTIR together with operando X-ray diffraction to investigate commercial Prussian Blue analogue electrodes for sodium-ion batteries. These measurements reveal distinct water dynamics in FeFe and MnFe systems and establish direct correlations between hydration state, structural evolution, and electrochemical response under practical high-loading conditions.[2] Finally, *operando* XAS studies will illustrate the mechanistic understanding of redox activity in emerging amorphous coordination polymers for versatile cation storage.[3] Beyond the scientific results, the talk will highlight operando cell design, instrumental considerations, studies on the effects of radiation damage, and experimental parameters required to obtain reliable mechanistic information.[4]

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OPERA Workshop
From 28 September to 2 October 2026
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A Case Study on NMC622: Developing a Multimodal Operando Metrology and Modelling Framework for Mechanistic Insights

Maria Alfredsson[1], Chris Vijeu[1], Grace Elliott Sherratt[2], Yvonne Grunder[2], Paul Thompson[2,3], Markys Cain[4], Erik Kelder[5], Pau Tarachiu[2] and Furio Cora[2]

[1]*University of Kent, School of Natural Sciences, Canterbury, UK*
[2]*University of Liverpool, Department of Physics, Liverpool, UK*
[3]*BM28, ESRF, Grenoble, UK*
[4]*Electrosciences Ltd, Farnham, Surrey, UK*
[5]*Technical University Delft, School of Natural Sciences, Delft, The Netherlands*
[6]*University College London, Department of Chemistry, London, UK*
Corresponding author: *[m.l.alfredsson@ikent.ac.uk]*

This work develops a multimodal operando metrology and modelling framework to capture the linked structural, electronic, and electrochemical changes that occur in battery materials during cycling. Although lithium nickel manganese cobalt oxides, $LiNi^xMn^yCo^zO^2$ (NMC), have been widely studied [e.g. 1], important questions remain regarding how nickel content governs their properties and degradation behaviour. Building on work initiated under OpMetBat (Operando Metrology Battery) and continued under HyMetBat (Hybrid Metrology Battery) [2], the current project applies a systematic characterisation strategy centred on a custom operando cell ("HZB-cell") designed for both in-house laboratory measurements and central-facility experiments. This cell enables direct comparison with conventional coin- and pouch-cell data. In this presentation we focus on multimodal X-ray diffraction (XRD) and X-ray absorption spectroscopy (XAS) measurements, although the broader study also incorporates Raman spectroscopy, pair distribution function (PDF) analysis, X-ray computed tomography (XCT), X-ray fluorescence (XRF), and X-ray Raman scattering (XRS).

Our approach is illustrated through a case study on a $LiNi^{0.6}Mn^{0.2}Co^{0.2}O^2$(NMC622)/*Graphite*(C) full cell. NMC622 is selected as a practical compromise between high nickel content and reduced sensitivity to ambient humidity, improving control over synthesis, handling, and measurement conditions, which is critical for building a reliable metrology-driven database.

Hybrid XAS/XRD/electrochemistry measurements reveal that during the first charge, the onset of Li^+-ion diffusion is accompanied by **large, rapid fluctuations in the $Ni^{2+}/Ni^{3+}/Ni^{4+}$ redox states**, whereas the XRD patterns exhibit **smooth, continuous bulk structural evolution**. This contrast demonstrates that **Li-ion mobility is non-linear and governed by highly localised electronic and cation-rearrangement events**, rather than by abrupt changes in the average crystal structure. These localised redox dynamics correlate with the formation of Ni^{2+} anti-sites. The combined measurements also help distinguish intrinsic structural changes from possible beam-damage artefacts and allow cathode behaviour to be correlated directly with the graphite anode. Atomistic simulations are employed both to support interpretation of the experimental data and, when combined with machine-learning analysis tools, to extract hidden physical relationships from the multimodal datasets.

To conclude, our multimodal measurements indicate a **decoupling between local electronic structure and bulk structural evolution during cycling**. Consequently, the machine-learning models currently under development must incorporate **non-linear valence descriptors**, rather than relying solely on bulk-averaged structural parameters.

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Accelerated, Interpretable Operando Impedance Characterization for Solid-State Batteries

Jake Huang[1], Alina Häußler[1], Dylan Thöle[1], Wolfgang Zeier[1,2]

[1]University of Münster, Institute for Inorganic and Analytical Chemistry, Münster, Germany

[2]Forschungszentrum Jülich GmbH, Institute of Energy Materials and Devices Helmholtz-Institute (IMD-4), Münster, Germany

Corresponding author: jake.huang@uni-muenster.de

Electrochemical impedance spectroscopy (EIS) is a key tool for investigating transport, interfaces, and degradation in solid-state batteries (SSB). However, its application is often limited by restrictive stability requirements, long measurement times, and ambiguous analysis. Here, we show how an accelerated impedance measurement protocol can mitigate instability, enable high-throughput *operando* data collection, and improve interpretability. The core technique combines time- and frequency-domain data through a distribution of relaxation times (DRT) transformation, enabling robust impedance characterization with ≥10-fold acceleration[1,2]. This enables EIS under previously inaccessible conditions: the rapid speed permits *operando* measurement to low frequencies (10 mHz) at high currents (1 C). High-throughput spectra can be collected in customized experiments, which allow machine learning analyses that can help disentangle impedance features and decouple experimental influences. The technique is demonstrated with cells based on $LiNi^{0.83}Co^{0.06}Mn^{0.11}O^{2}$ and $Li^{6}PS^{5}Cl$, which enables separation of electrode-specific impedance features and the identification of kinetic bottlenecks. The approach could have versatile applications in SSB: fast insight into interfacial stability and kinetics for materials screening; charging profile optimization guided by real-time EIS; multimodal *operando* experiments linking impedance features to distinct materials properties; and autonomous AI-driven measurement systems[3]. Importantly, the foundational measurement technique is system-agnostic and can be applied to diverse systems, ranging from batteries to electrolyzers to solar cells.

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Operando XRD: From synchrotron to laboratory

Peter Siffalovic[1,2], Erik Simon[1,2], Karol Vegso[1,2], Arslan Raza[2], Soundarya Neelanarayanan[2], Poongodi Ayyanusamy[2], Anna Kalosi[2], Shuang Deng[2], Rangaraj Gomathi[2], Aditya Pandey[2]

[1]*Centre for Advanced Materials Application, Slovak Academy of Sciences, Bratislava, Slovakia*

[2]*Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia*

Corresponding author: *peter.siffalovic@savba.sk*

Operando characterization of solid-state batteries (SSBs) in real time is essential because it provides rapid feedback on how to improve their performance. Operando XRD/GEIS is particularly powerful in this respect, as it combines electrochemical insight into the active components with structural characterization of the phases present. This combination is especially valuable when electrochemical performance declines, allowing the loss of performance to be correlated with specific phase changes.

Currently, the most advanced operando XRD/GEIS analysis is performed at synchrotron facilities, utilizing high-brilliance, high-energy X-rays. I will showcase this technique using SSBs with NMC cathode active material. However, improving SSB properties requires the ability to perform operando XRD/GEIS regularly. I will demonstrate that a comparable setup can also be used in laboratory settings. This setup's capabilities will be illustrated through tests on various SSBs, including those with sulfide and halide solid-state electrolytes, combined with intercalation cathodes like LMFP and NMC, as well as conversion cathodes such as sulfur.

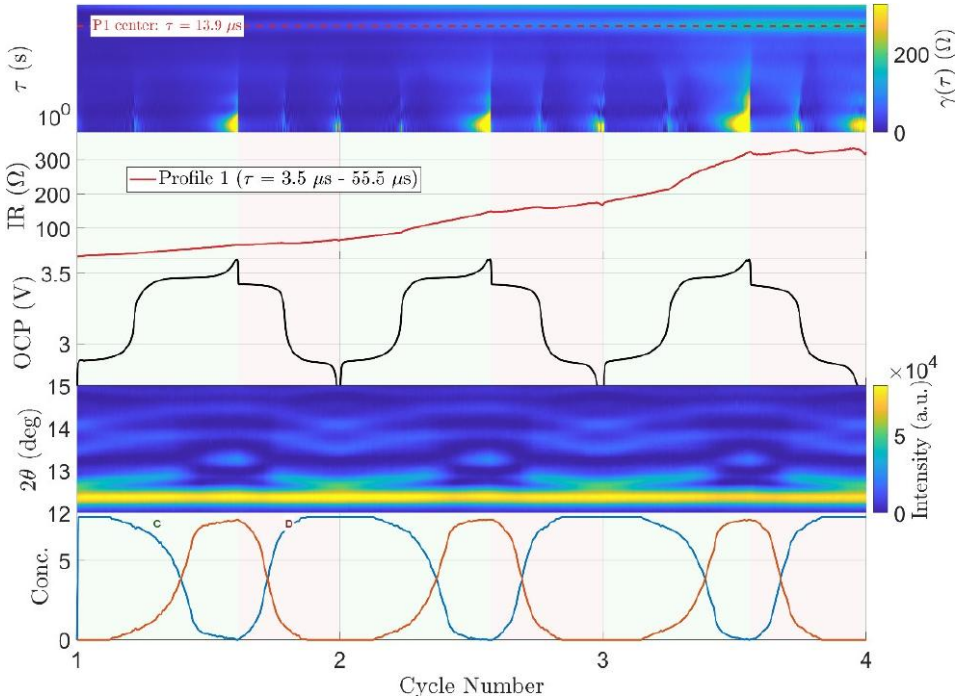


Figure 1. *An example of multimodal operando XRD/GEIS evaluation of LMFP/LIC SSBs*

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Garnet-Based Solid-State Li Metal Batteries

Dr. Venkataraman Thangadurai[1]
[1]School of Chemistry, University of St Andrews, Scotland, UK

Renewable energy sources such as solar and wind are vital for reducing greenhouse gases and transitioning to a decarbonised economy. Because they are intermittent, reliable storage and conversion systems are essential. Electrochemical devices, including rechargeable batteries and fuel cells, store electricity and convert waste into chemicals. Lithium-ion batteries (LIBs) are widely used in transport, but they have limitations. Current organic electrolytes have issues such as flammability, stability, and toxicity; thus, research is focusing on thermally stable ceramic electrolytes and cost-effective sodium-ion batteries. Next-generation solid-state membranes and elemental metal electrodes aim to enable safe, high-energy, durable batteries. This talk covers advanced Li-stuffed garnet-based membranes and solid-state Li metal batteries.

Biography: Dr Venkataraman Thangadurai is a full professor and Chair in Energy at the School of Chemistry. He is a Faraday Adjunct Professorial Fellow at the University of St Andrews. He is a Fellow of the Royal Society of Chemistry (UK), the Royal Society of Canada, and the Electrochemical Society (USA). He has published more than 286 peer-reviewed journal articles (H-index: 74). He received the Keith Laidler Award from the Canadian Chemical Society (CSC) in 2016 and the Research Excellence Award in Materials Chemistry from CSC in 2021. He has also received the Battery Division Research Award from the Electrochemical Society in 2025. His research activities include the discovery of novel solid-state electrolytes exhibiting fast lithium, sodium, and proton conduction, as well as electrodes for both advanced solid-state metal batteries and solid oxide fuel cells.

Sulfide solid electrolytes: kinetic limitations in composite cathodes and the path towards commercialization

Kristian Nikolowski[1], Silian Yanev[1], Henry Auer[1], Christian Heubner[1], Mareike Partsch[1], Alexander Michaelis[1,2]

[1]*Fraunhofer Institute for Ceramic Technologies and Systems IKTS, Dresden, Germany*
[2]*Chair of Inorganic Non-Metallic Materials, Technische Universität Dresden, Germany*
Corresponding author: *kristian.nikolowski@ikts.fraunhofer.de*

In sulfide-based all-solid-state batteries (ASSBs), the composite cathode is where energy and power density compete with each other. A high fraction of active material (AM) is needed for high energy density, but it leaves little solid electrolyte (SE) for Li^+ transport. Transport through the SE and solid-state diffusion inside the AM are coupled through the microstructure and the AM-SE contact area, and which of them limits a given cathode is often unclear. Without that information, it is hard to say whether SE conductivity or contact area is the more promising parameter.

We use chronoamperometric (CA) discharge at a fixed cut-off voltage to separate the two. A single CA step covers a continuous range of rates and gives the same capacity-rate information as a galvanostatic test in a fraction of the time [1]. Fitting the curve with a power-law decay yields an exponent *n* that distinguishes resistive ($n \approx 1$) from diffusive ($n \approx 0.5$) limitation. We validated *n* against effective ionic conductivities from impedance spectroscopy on cathode-symmetric cells and against apparent Li^+ diffusion coefficients from the galvanostatic intermittent titration technique (GITT).

The study covers $LiNi^{0.8}Co^{0.1}Mn^{0.1}O^2$ (NCM811) and Li^6PS^5Cl (LPSCl) cathodes with AM fractions from 51 to 90 wt%, polycrystalline granular versus single-crystalline NCM811, and as-received versus ball-milled LPSCl [2]. Across this range *n* falls from ≈ 1.0 to ≈ 0.4, so the limitation shifts from resistive to diffusive. The shift of the limiting mechanism is attributed to differences in the AM-SE contact area. Referenced to liquid-electrolyte cells with the same AM, the SE-covered fraction of the AM surface falls from about 85 % in the SE-rich single-crystal cathode to 3 % at 90 wt% AM. Single crystals reach the highest AM utilization but become diffusion-limited above 84 wt%. Ball-milled LPSCl improves both effective conductivity and coverage, even though its bulk conductivity is only half that of the as-received powder.

Two further cases put this in perspective. Between 50 and 400 µm cathode thickness, *n* falls only from ≈ 0.95 to ≈ 0.80, together with a rise in area-specific resistance after cycling, which points to contact loss from AM volume change. Compaction pressure leaves *n* between ≈ 0.97 and ≈ 1.03. Both effects are small next to the composition [3].

Translated into an idealized cell, the calculated gravimetric energy density does not rise monotonically with AM content but peaks at intermediate fractions. Ball-milled LPSCl shifts that peak to higher AM content and raises it, at 0.1C from 375 to 405 Wh kg^{-1} [3]. The SE particle size, not the bulk conductivity of the SE, decides where the optimum sits. The CA workflow resolves resistive and diffusive limitation fast enough to screen microstructure concepts and to supply parameters for transport models.

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Glass and Glass-Ceramic Composite Electrolytes for Enhanced and Stable Interfaces with Lithium Metal

Nataly Carolina Rosero-Navarro[1]

[1]Department of Glass, Institute of Ceramic and Glass (ICV-CSIC), Kelsen 5, 28049 Madrid, Spain

Corresponding author: rosero@icv.csic.es

The development of all-solid-state batteries with lithium-metal anodes requires solid electrolytes that combine fast Li-ion transport with chemical, electrochemical, and mechanical stability at the electrode/electrolyte interfaces. Although crystalline ceramic electrolytes offer high ionic conductivity, their rigid solid-solid contacts and grain boundaries can generate large interfacial resistance and preferential pathways for lithium penetration. Glasses provide a complementary platform because their composition, network structure, and interfacial chemistry can be continuously tailored, while glass-ceramic composites can combine these attributes with the transport properties and mechanical robustness of crystalline electrolytes.

This presentation will discuss our recent work on lithium borate and lithium phosphate glass electrolytes, with emphasis on how compositional modification controls Li-ion transport and, particularly, the stability of the interface with lithium metal. The incorporation of AlF^3 illustrates the strong dependence of interfacial behavior on the underlying glass network. Fluorine-containing modifications can alter network connectivity, lithium environments, and the chemistry developed during contact with lithium metal. Comparison between borate- and phosphate-based compositions shows that the effect of fluorination cannot be considered independently of glass structure and composition, providing useful guidelines for designing stable glass/Li interfaces.

A complementary strategy is the incorporation of nitrogen into lithium alumino-phosphate glasses. Substitution of oxygen by nitrogen generates P-N-containing structural units and modifies both network connectivity and the local environment of lithium ions. This approach provides a route to couple bulk ion transport with improved interfacial behavior. The relationship between nitrogen incorporation, Li-ion mobility, polarization during lithium plating/stripping, and the evolution of the glass/lithium interphase will be discussed, highlighting the role of glass-network chemistry in controlling interface processes.

Finally, these concepts will be extended to garnet-type $Li^7La^3Zr^2O^{12}$ (LLZO)-based solid electrolytes. In these materials, glass phases can act as functional grain-boundary modifiers and sintering additives, promoting densification and improved grain connectivity while modifying lithium transport across interfaces. This strategy complements other approaches based on amorphous, hybrid, and engineered inorganic interlayers aimed at mitigating chemical and mechanical degradation at solid-solid interfaces. The resulting microstructural and interfacial engineering is relevant to reducing interfacial resistance, suppressing lithium penetration, and improving cycling stability.

Together, these studies show that glass chemistry offers a versatile tool for engineering interfaces across different length scales, from local lithium coordination and the glass/lithium-metal interphase to grain boundaries in ceramic composites. Establishing composition-structure-transport-interface relationships in glasses and glass-modified garnets provides design principles for developing stable solid electrolytes and interfaces for next-generation all-solid-state lithium-metal batteries.

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OPERA Workshop
From 28 September to 2 October 2026
at La Cristalera in Miraflores de la Sierra (Madrid)

Progress in Electrodes for Thin-Film Batteries

E. Vasco[1], A. Galindo[1], A. Marchetti[1], A. Bouthayna[2], P. Hernandez[2], J. Diaz-Sánchez[2], E. López-Ortin[2], G. García[2] and C. Polop[2]

[1]*Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas*

[2]*Universidad Autónoma de Madrid*

Corresponding author: *enrique.vasco@csic.es*

Abstract *— I summarize our recent results on the preparation, optimization, and engineering of cathodes for alkali-ion batteries in thin-film, epitaxial, and blended configurations [1,2,3], as well as metallic anodes [4,5,6]. I also discuss current challenges in the fabrication of thin-film solid-state electrolytes by physical vapor deposition, together with recent advances in the characterization of thin-film batteries using HAXPES [6] and operando ion-beam analysis.*

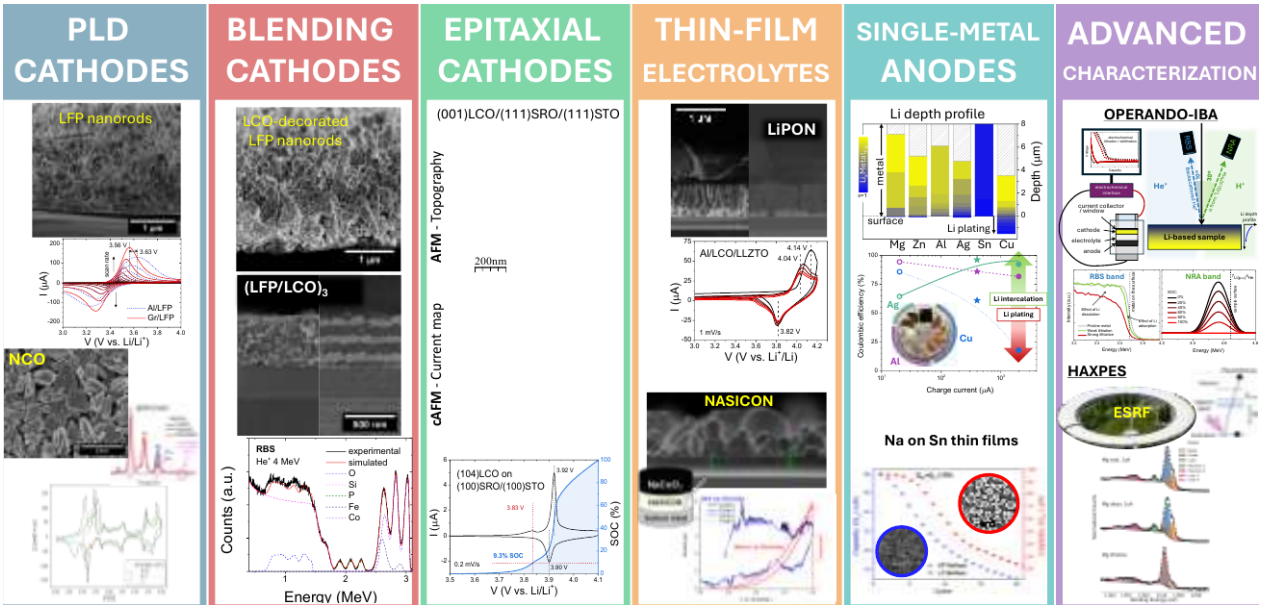


Figure 1. *Collage of the results from CSIC and UAM partners in the implementation of thin-film alkali-ion battery*

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OPERA Workshop
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Zn-air batteries investigated with complementary spectroscopy and imaging approaches

Benedetto Bozzini*, Alessandra Gianoncelli[2], Lucia Mancini[3], Francesco Nespoli[4]

[1] Department of Energy, Politecnico di Milano, via Lambruschini 4, 20156, Milano, Italy

[2] Elettra Sinctrotrone Trieste S.C.p.A., Strada Statale 14 - km 163,5 in AREA Science Park 34149 Basovizza, Trieste, Italy

[3] Slovenian National Building and Civil Engineering Institute (ZAG), Dimičeva ulica 12, SI-1000, Ljubljana, Slovenia

[4] Media Lario S.r.l., via al Pascolo 10, 23842, Bosisio Parini (LC), Italy

Corresponding author: benedetto.bozzini@polimi.it

Rational exploitation of the energy produced by renewable sources and electromobility, call for the development of **efficient and reliable energy storage** systems. Batteries are natural candidates for this purpose, and metal-air batteries are expected to gain momentum with respect to Li-ion technologies, because of their potentially higher energy density and sustainability. Among post-Li metal-air systems, **Zn-air batteries** are especially promising for safety, environmental and cost reasons. Disposable devices are already commercially available, but rechargeable systems are still far from the market, because two key challenges still remain open: on the one hand the optimization of **bifunctional catalysts** for the reversible air-cathode, that would increase the round-trip efficiency, and, on the other hand, the minimization of **anode degradation** in both the discharge and charge processes. Even if research is making great efforts in the field, satisfactory grasp of the mechanisms underlying these processes is still lacking. This talk will focus on an approach to the fundamental understanding of a comprehensive range of open issues of Zn-air batteries, based on **spectroscopic and imaging methods**, with special emphasis on ***in situ* X-ray** techniques. Recent results will be expounded, regarding: (i) **oxygen catalyst fabrication, operation and degradation**, followed **by soft-X ray microspectroscopies** (SXM) in the direct and Fourier spaces as well as EXAFS [1]; (ii) **unstable electrodeposition and dissolution** studied by SXM and **photoelectron microspectroscopy** [2] in different electrolytes [3]; (iii) **shape change of Zn anodes** investigated by ***in situ* X-ray micro Computed Tomography** [4]. This multi-technique approach, combined with mathematical modelling of electrochemical phase formation and device cycling [5], opens up new routes for knowledge-based cathode and anode material design and the definition of rational charge/discharge policies.

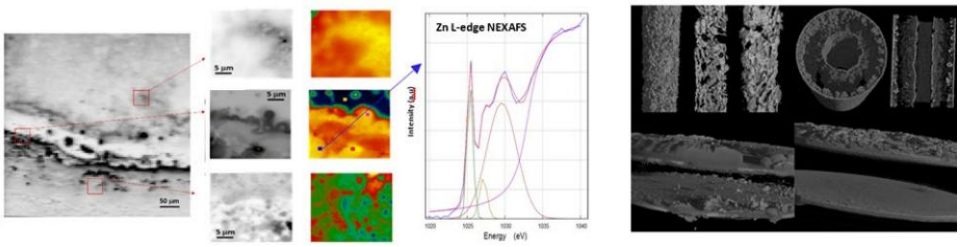


Figure 1. Representative selection of in situ spectal and tomographic imaging of RZAB electrodes.

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Ion beam analysis: a tool for battery research and beyond

Gastón García López[1]

[1]*Centro de Micro-Análisis de Materiales, Universidad Autónoma de Madrid, Madrid, Spain*

Corresponding author: *gaston.garcia@uam.es*

Ion beam techniques are a powerful analytical and processing tool for advanced materials research. These set of techniques, known as IBA (for Ion Beam analysis) will be presented, taking the Center for Micro-analysis of Materials (CMAM), at UAM, as reference background [1]. Emphasis will be made on possibilities of interest for battery research. IBA provides an insight complementary to other analytical tools, mainly via depth profiling of the Li content in thin samples, via the Nuclear Reaction Analysis (NRA) technique. The principle behind this approach will be introduced, and capabilities and limitations will be discussed, including the prospect of advancing towards operando experiments.



Figure 1. *Picture of the ion accelerator at CMAM*

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AI assisted multiscale modelling of metal anode-electrolyte interfaces in solid state batteries

Neubi Xavier[1], Yuheng Du1, Tao Chen[1], Qiong Cai[1]

[1]*School of Chemistry and Chemical Engineering, Faculty of Engineering and Physical Sciences, University of Surrey, Guildford GU2 7XH, United Kingdom*

Corresponding author: *q.cai@surrey.ac.uk*

Zero-excess solid-state Li batteries (SSLBs) are promising next-generation batteries, due to their high theoretical energy density and simplified manufacturing process by eliminating highly reactive Li metal at the fabrication stage. However, the formation and growth of Li dendrite during battery cycling cause significant capacity fade and fatal battery failure [1,2]. Within the OPERA project, we use AI assisted multiscale computational modelling to help design the metal anode-electrolyte interfaces, to enhance the safety and performance of zero-excess SSLBs.

Interlayer metals could potentially help achieve stable Li deposition/stripping process, suppressing Li dendrite formation. Using density functional theory simulations, a relationship between the Li deposition overpotential and diffusion barriers is established to help identify interlayer metals that can enable efficient Li deposition [3]. We also collaborate with experimental partners to design a Sn-modified copper substrate, which forms alloying reaction with Li to yield a deposition interlayer composed of Sn and Li-Sn intermetallics that regulates both Li diffusivity and adsorption during initial deposition, leading to enhanced battery performance [4]. Importantly, we combine fine-tuned machine-learning interatomic potentials (MLIP) with large-scale molecular dynamics (MD) simulations to resolve the atomistic pathways of lithium alloying and crystallization on Cu and interlayer metals. Zn and Mg show alloy-mediated crystallization process to enhance lithium diffusion and structural uniformity, whilst the Li nucleation on Cu and the formation of intermetallic alloys with Bi are revealed [5]. These results are validated by experimental observations through scanning electron microscopy, X-ray diffraction, atomic force microscopy, and time-of-flight elastic recoil detection corroborates the predicted alloying and phase evolution. The MLIP enhanced MD simulations are also performed for metal anode-solid state electrolytes (SSEs), revealing the formation of different interphase compounds when different SSEs and different interlayer metals are used. Our modelling framework can help design metal interlayers for regulating lithium nucleation and enabling safe operation of next-generation lithium batteries. We have also carried out meso-scale computational phase-field analysis of the Li dendrite growth at the Li/LLZO interface, assuming preferential propagation along the GB pathways of the polycrystalline LLZO solid electrolyte. Reducing the interfacial reaction rate is demonstrated to be a substantially more effective suppression strategy than increasing external stacking pressure, highlighting interfacial engineering as the priority design lever for next-generation ASSLB development. Machine learning surrogate models are then used to predict Li dendrite growth in LLZO considering various influential factors.

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Participant List

All confirmed participants - invited seniors, OPERA seniors and junior researchers

INVITED SENIORS

Maria Alfredsson
University of Kent
m.l.alfredsson@kent.ac.uk

Ashley Black
Instituo de Ciencia de Materiales de Barcelona CSIC
ablack@icmab.es

Benedetto Bozzini
Politecnico di Milano
benedetto.bozzini@polimi.it

Rosalía Cid Barreno
CIC energiGUNE
rcid@cicenergigune.com

Juan de la Figuera
Instituto de Química Física Blas Cabrera CSIC
juan.delafiguera@csic.es

Santhana Eswara Moorthy
Luxembourg Institute of Science and Technology
santhana.eswara@list.lu

Till Fuchs
Justus Liebig University Giessen
Till.Fuchs@uni-giessen.de

Gastón García López
Autonomous University of Madrid
gaston.garcia@uam.es

Chun Ann Huang
Imperial College London
a.huang@imperial.ac.uk

Jake Huang
University of Muenster
jake.huang@uni-muenster.de

Juan Miguel López del Amo
CIC energiGUNE
jmlopez@cicenergigune.com

Carolina Rosero-Navarro
Instituto de Ceramica y Vidrio CSIC
rosero@icv.csic.es

Venkata Thangadurai
University St-Andrews
vt36@st-andrews.ac.uk

OPERA SENIORS

Manfred Burghammer
ESRF synchrotron
burgham@esrf.fr

Qiong Cai
University of Surrey
q.cai@surrey.ac.uk

Tao Chen
University of Surrey
t.chen@surrey.ac.uk

Michael Foerster
ALBA synchrotron
mfoerster@cells.es

Enrique Garcia Michel
Autonomous University of Madrid
enrique.garcia.michel@uam.es

Stephan Junker
Eurogrant GmbH
stephan.junker@eurogrant.de

Carmen Morant Zacarés
Autonomous University of Madrid
c.morant@uam.es

Kristian Nikolowski
Fraunhofer IKTS
kristian.nikolowski@ikts.fraunhofer.de

Miguel Angel Niño Orti
Instituto de Química Física Blas Cabrera CSIC
manino@iqf.csic.es

Celia Polop Jordá
Autonomous University of Madrid
celia.polop@uam.es

Herko P. van der Meulen
Autonomous University of Madrid
herko.vandermeulen@uam.es

Peter Siffalovic
Centre for Advanced Materials Application SAS
siffalov@gmail.com

Enrique Vasco Matias
Instituo de Ciencia de Materiales de Madrid CSIC
enrique.vasco@csic.es

JUNIOR RESEARCHERS

Christian Ahlers
Eurogrant GmbH
christian.ahlers@eurogrant.de

Yondriel de Armas Figueroa
Instituo de Ciencia de Materiales de Madrid CSIC
yondriel.dearmas@estudiante.uam.es

Jesús Díaz-Sánchez
Autonomous University of Madrid and Instituo de Ciencia de Materiales de Madrid CSIC
jesus.diazs@uam.es

Yuheng Du
University of Surrey
yd0007@surrey.ac.uk

Kalina Fornal
Instituto de Química Física Blas Cabrera CSIC
kfornal@iqf.csic.es

Clara Gutiérrez Cuesta
Instituto de Química Física Blas Cabrera CSIC and Universidad Complutense de Madrid
clagut02@ucm.es

Pablo Hernández Martín
Autonomous University of Madrid
pablo.hernandezm@uam.es

Natalia Kwiatek-Maroszek
ALBA synchrotron
nkwiatek@cells.es

François Liénard
ESRF synchrotron
francois.lienard@esrf.fr

Emma López Ortín
Autonomous University of Madrid and Instituo de Ciencia de Materiales de Madrid CSIC
emma.l.ortin@gmail.com

Andrea Marchetti
Instituo de Ciencia de Materiales de Madrid CSIC
andrea.marchetti@csic.es

Ange Maurice
Autonomous University of Madrid
ange.maurice@uam.es

Soundarya Neelanarayanan
Centre for Advanced Materials Application SAS
nssow1998@gmail.com

Melike Nur Yildirim
University of Surrey
melikeny1@gmail.com

Alejandro Ramo Irurre
Instituo de Ciencia de Materiales de Barcelona CSIC
aramo@icmab.es

Sayantan Sharma
Luxembourg Institute of Science and Technology
sayantan.sharma@list.lu

Karol Vegso
Centre for Advanced Materials Application SAS
karol.vegso@savba.sk

Zachary Warren
Instituto de Ceramica y Vidrio CSIC
warren@icv.csic.es