OPERA

Development of Operando Techniques and Multiscale Modelling to Face the Zero-Excess Solid-State Battery Challenge

Presented by:

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BATTERY 2030+

Project Overview

UAM Universidad Autónoma de Madrid

Celia Polop, Carmen Morant, Enrique G. Michel, Herko vd Meulen

Coordination. Scanning probe microscopies.
Synchrotron radiation photoelectron spectroscopies.

MONTAN UNIVERSITÄT LEOBEN

Jozef Keckes, Christoph Gammer

Synchrotron X-ray nano-diffraction. Transmission electron microscopy.

CEMEA

Peter Siffalovic

Synchrotron radiation X-ray scattering. Raman spectroscopy.

ALBA

Miguel Angel Niño, Michael Foerster

Synchrotron photoemission electron microscopy.
Low energy electron microscopy.

ESRF The European Synchrotron

Manfred Burghammer

Synchrotron radiation X-ray diffraction

NTNU

Daniel Rettenwander, Mir Mehraj Ud Din

Li-based bulk materials development. Cell design.
Electrochemical analysis. Electron backscatter diffraction.

UNIVERSITY OF SURREY

Qiong Cai, Tao Chen

Modelling and theory

Fraunhofer IKTS

Kristian Nikolowski

Na-based bulk materials development. Electrochemical analysis.

AVL

Simon Erker, Filip Maletic

Modelling and simulations

CSIC Consejo Superior de Investigaciones Científicas

Enrique Vasco, Juan Rubio

Thin-film materials development. Cell design. Electrochemical analysis. Synchrotron photoelectron spectroscopies.

huber scientific

Tobias Huber

Development of devices

EUROGRANT

Stephan Junker, Christian Ahlers

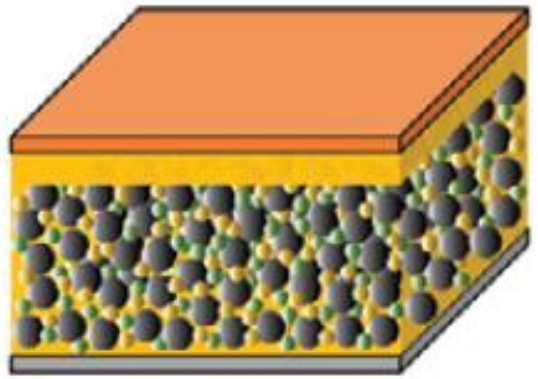
Administrative management.
Communication. Dissemination.

Top Goals

What happens during the initial state of anode formation in Zero-Excess Solid-State Li and Na Batteries?

How can we tailor the nucleation and growth of the anode?

ZESSB



Nanoscale multiparameter operando mapping of the battery interfaces:
stress field, microstructure, phase distribution, chemical composition, oxidation state, impedance, degradation.

Development of novel operando synchrotron techniques at ESRF, ALBA and DESY with nanometer resolution.
Multiscale modelling assisted by a machine learning framework.

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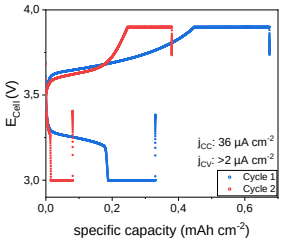
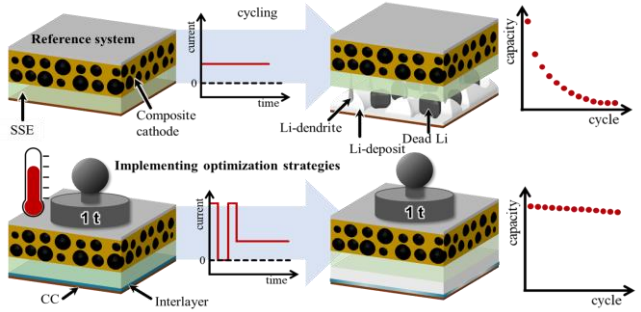
Short First Results

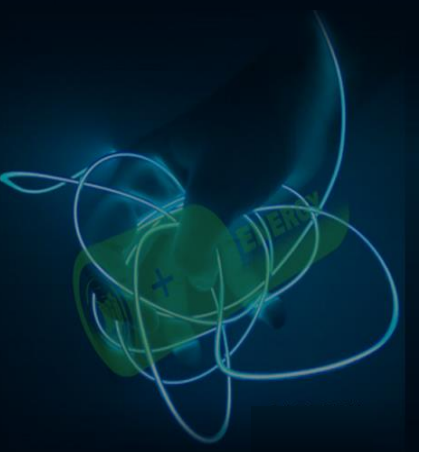
- Thin-film solid-state cell development for high-resolution 4D investigations
- Operando microscale spatio-temporal tracking of stresses and interfaces for ZESSBs
- Development of an operando stacking-pressure stage for nano-XRD at ID13-ESRF
- Operando microscale spatio-temporal tracking of stresses and interfaces for ZESSBs
- Development of an operando stacking-pressure stage for nano-XRD at ID13-ESRF
- Operando cross-sectional nano-XRD & post-mortem analysis of Li-ZESSBs
- Development of an operando bending-strain stage for photoelectron spectroscopy at ALBA and ESRF
- Operando Low Energy and Photo Emission Electron Microscopy (LEEM-PEEM) and AFM of Na and Li-ZESSBs
- A modelling framework for screening interlayer materials
- Nuclear Reaction Analysis for screening interlayer materials
- Coupled Electrochemical-Mechanical Modelling of a SSB Cell
- Reference cell design

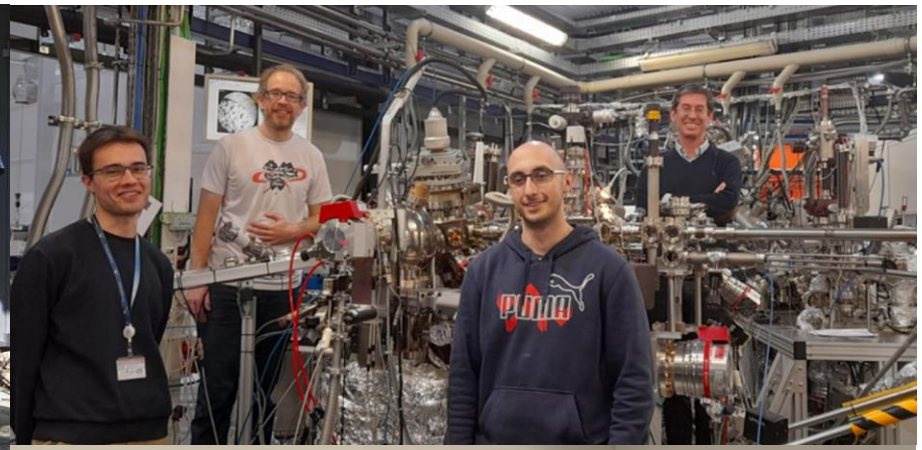


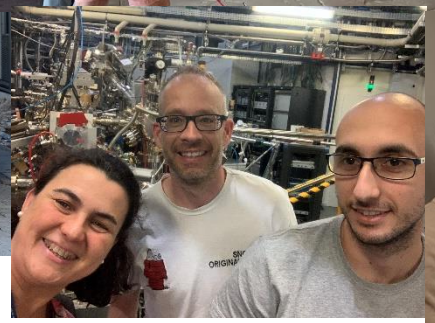


Alignment with the Roadmap Goals

- **One of the important aspects of OPERA is a development of methodology and frameworks for modelling of advanced cell designs**
- **Atomistic-scale, first-principle models → screening of materials, understanding of underlying phenomena**
- **Continuum-scale, cell-level models → simulation of a final product, design optimization**
- **Simulation benefits:**
  - Material development
  - Design optimization
  - Understanding the limits
- **We would suggest that the future Roadmap reflects the possible benefits of using the advanced simulation techniques for a development of new battery technologies**







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