# SiGNE Project


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This project has received funding from the European Union's Horizon Europe transport programme under grant agreement No 101069738

# SiGNE Objectives

- New Li-ion Cell Chemistry
- Modelling Guided Material Design & Synthesis
- Mechanistic Insight, Boosted Performance
- Prototype Validation BMS Development
- Cost-Effective Cells <€80/kWh
- Production and Ownership in Europe
- Sustainability, Circular Economy, Recycling

## Performance:

- Prototype Demonstration at TRL6
- Demonstrate High Energy Density
- Fast Charging Capability
- Extended Cycle Life & Stability
- High Residual Energy for 2nd Life Users
- High Materials Recovery & Recycling

## Impact:

- Increased European Battery Competitiveness
- Increased EV Range & Uptake
- Reduced EV Consumer Costs
- Aid Sustainable Supply Chain
- Transport Sector GHG Reduction

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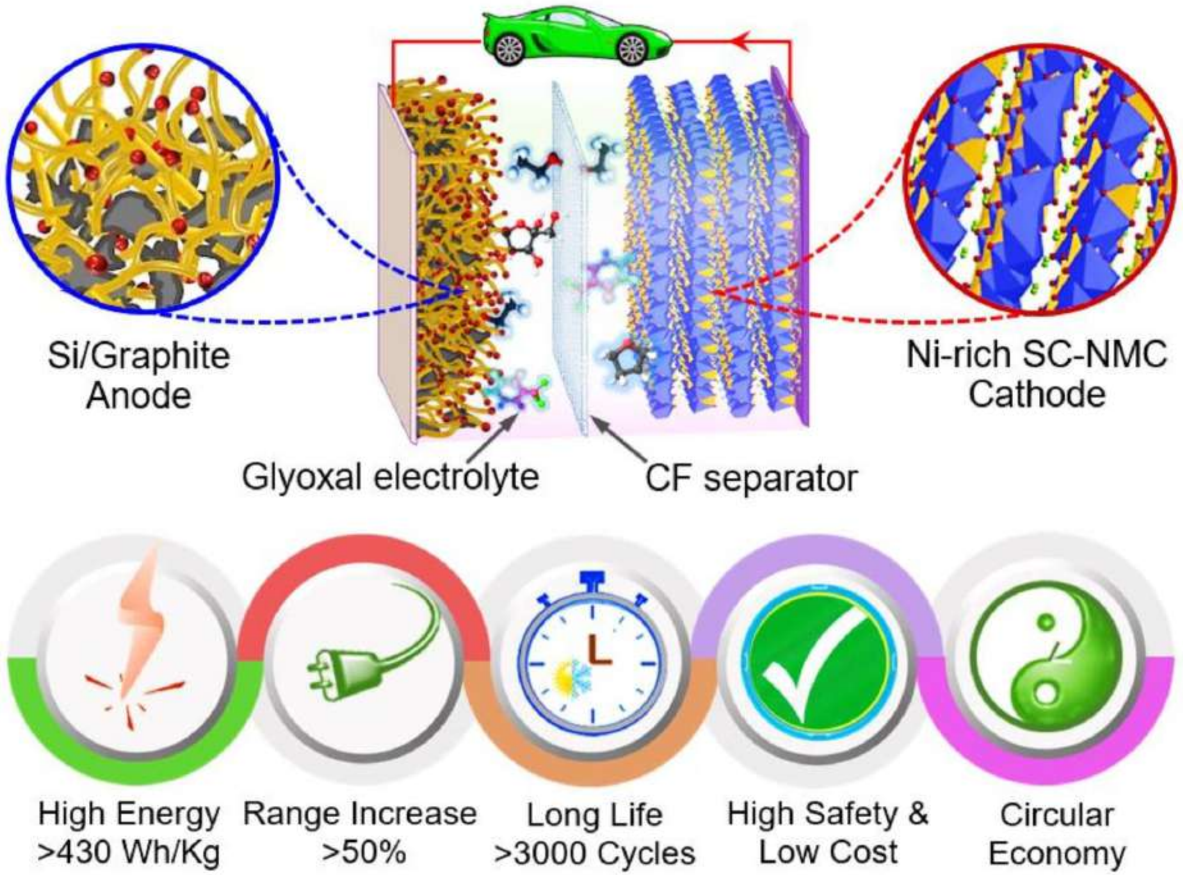
# SiGNE Chemistry & Targeted Features




| | SoA | SiGNE 1 | SiGNE 2 | SiGNE 3 |
|---|---|---|---|---|
| Cathode composition | NMC622 | Ni-rich NMC | Ni-rich NMC | Ni-rich NMC |
| Anode - Si wt. fraction | 0 | 0.2 | 0.3 | 0.3 |
| Anode - Gr wt. fraction | 1 | 0.8 | 0.7 | 0.7 |
| Si Capacity (mAh/g) | 0 | 1500 | 2000 | 2500 |
| Gr Capacity (mAh/g) | 360 | 360 | 360 | 360 |
| Total Anode Capacity (mAh/g) | 360 | 588 | 852 | 1002 |
| Anode Porosity (%) | 25 | 35 | 45 | 45 |
| Specific Energy Density (Wh/kg) | 289 | 340 | 390 | 433 |
| Specific Power (W/kg) | | 680 | 780 | 2598 |
| Volumetric Energy Density (Wh/L) | 745 | 872 | 995 | 1110 |
| Relative EV Range (%) | 100% | 118% | 135% | 150% |

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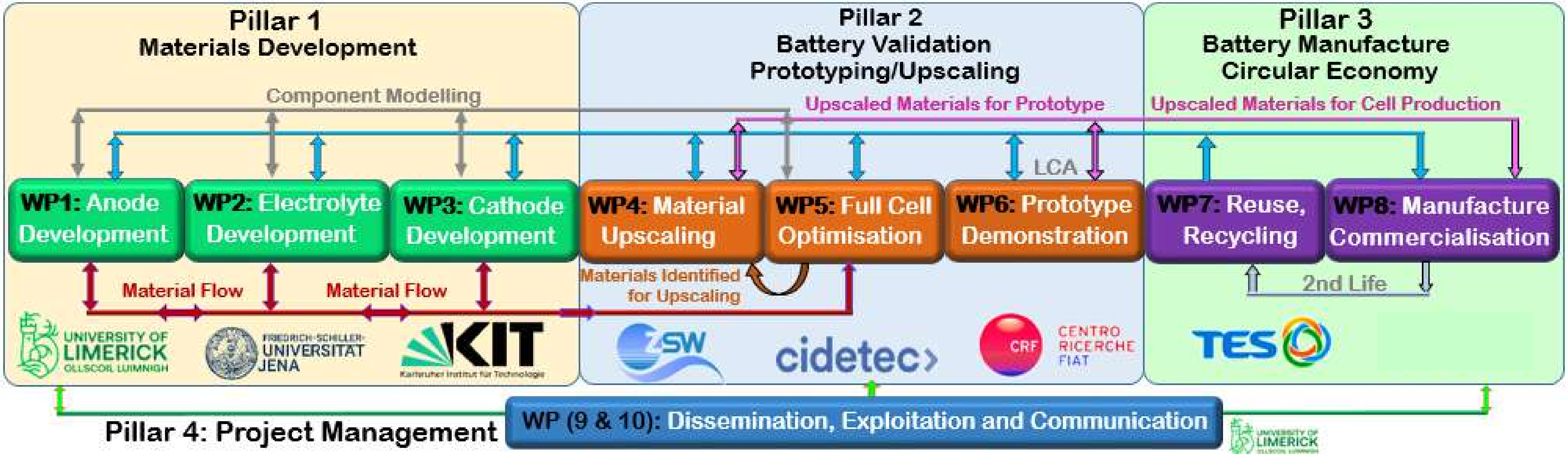
# SiGNE Project Layout and Interactions

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# Si Anode Development

## Target and Motivation

***Development of Si NW/graphite composite materials to increase anode specific capacity.***

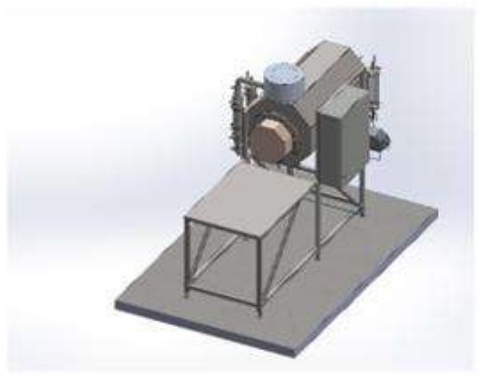
- Si incorporation at 20-30 % can significantly increase cell level energy density.

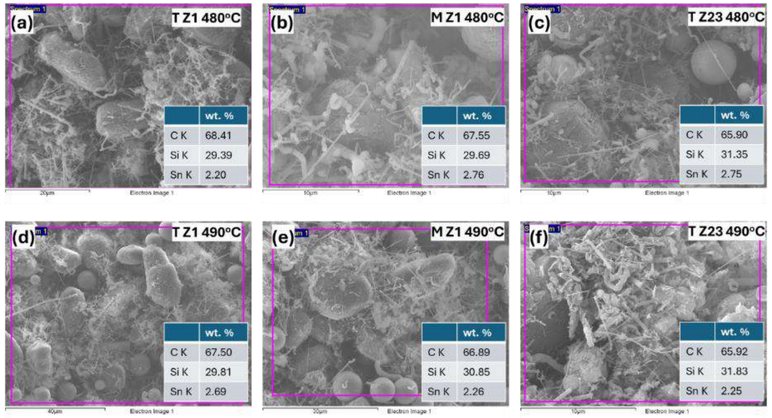
## Approach

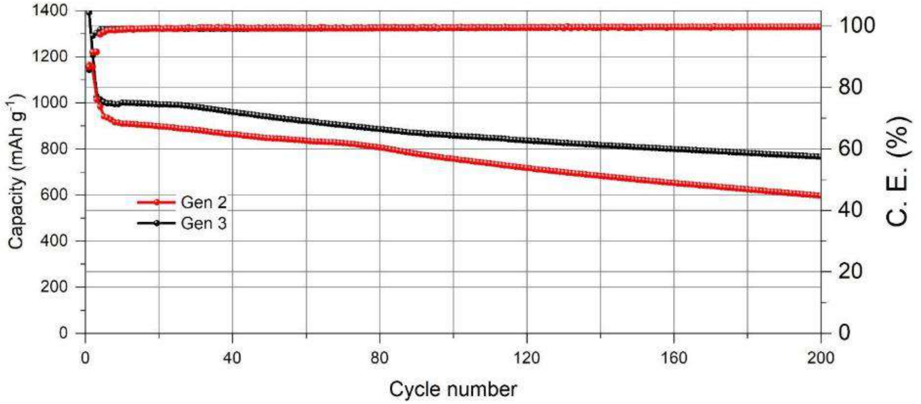
- Direct growth of Si NWs from graphite using Sn as a seed in a wet chemical approach. Optimise reaction conditions for upscaling to kg scale. Optimise Sn dispersal for NW diameter and Si % control. Controlled prelithiation of the anode is being investigated to mitigate early cycle Li inventory losses by **SID**.

## Progress & Challenges

- Gen 2 and Gen 3 anode materials have been developed, with specific capacities >1000 mAh/g achieved.
- Batch % continuous reactors under development. Hurdles linked to reactor development, well underway.



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# Electrolyte Development

## Target and Motivation

***A new generation of glyoxal-based electrolytes (tetramethoxy glyoxal (TMG)/tetraethoxy glyoxal (TEG)).***

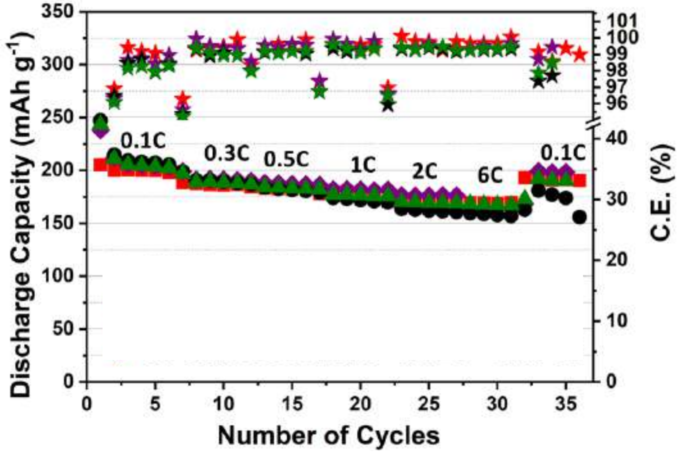
- Higher safety electrolytes with interphase control ability are required for high energy cells. Glyoxal electrolytes can increase thermal stability/boiling point and decrease flammability, with flexibility for different formulations.

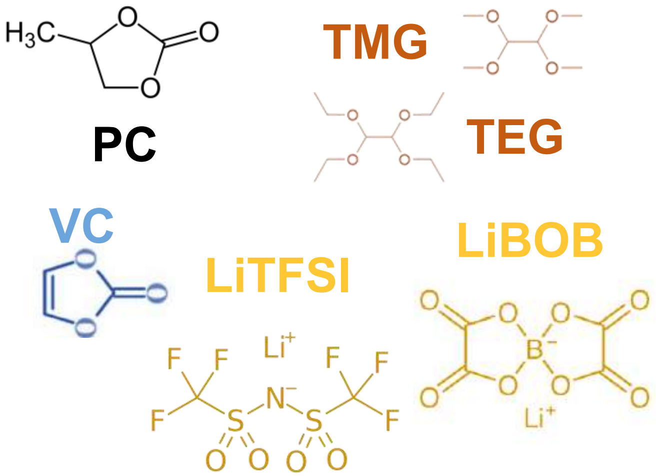
## Approach

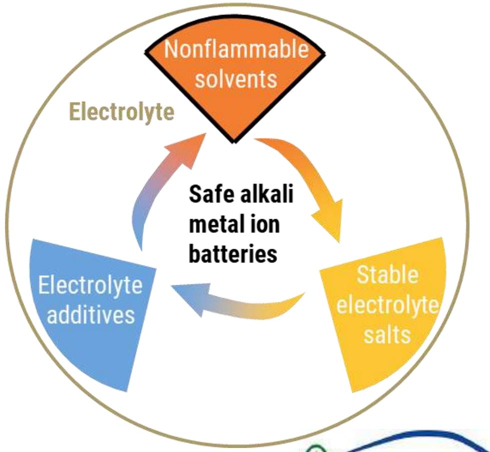
- Optimize glyoxal:propylene carbonate (**PC**) with imide-based Li salts, (e.g., **LiTFSI** and **LiFSI**).
- SEI controlling additives to such as (**VC, VEC, FEC**) and dditives to mitigate anodic dissolution (**LiBOB**)

## Progress & Challenges

- Gen 2 electrolytes have been identified with optimized solvent/salt/additive composition. Promising high-rate performance with Gen 2 cathode material and with Si/Gr anodes. Possible reactivity with cell casings have been identified (SS/Cr).

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# Separator Concept

## Target & Motivation

***Develop a micro/nanoscale cellulose fibre separator with high thermal stability/improved safety.***

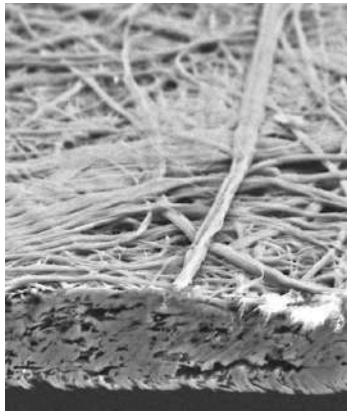
- High mechanical strength and compression resilience is required to facilitate Si-anode volume expansion.

## Approach

- Interconnected porous structure by using micro- and nano-scaled fibres to allow for fast ion exchange and high rate capability

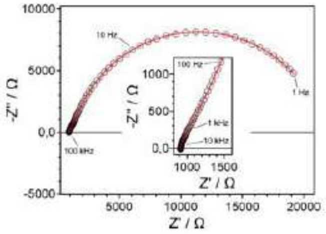
## Progress & Challenges

- Gen 2 separator with optimised thickness achieved. Ongoing work on impedance analysis (MacMullin number).
- Current efforts are working towards improving the porosity of the separator.



$$N_M = \frac{\kappa}{\kappa_{eff}} \qquad N_M = \frac{\tau}{\varepsilon} = \frac{R_{Ion} \cdot A \cdot \kappa}{d}$$

| Symbol | Name | Unit |
|---|---|---|
| $N_M$ | MacMullin number | - |
| $\kappa$ | electrolyte conductivity | mS/cm |
| $\kappa_{eff}$ | effective electrolyte conductivity in porous medium | mS/cm |
| $\varepsilon$ | porosity of porous medium | - |
| $\tau$ | tortuosity of porous medium | - |
| $d$ | length | µm |
| $R$ | resistance | Ω |
| $A$ | area | $cm^2$ |

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# SC-NMC Cathode Development

## Target & Motivation

***Development of Ni-rich/Co-poor, single-crystalline NMC with direct recycling suitability.***

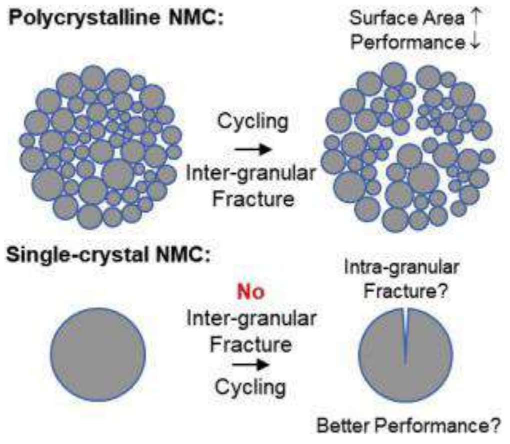
- Reduced surface area reduces electrolyte decomposition. High discharge voltage unlocks high energy density

## Approach

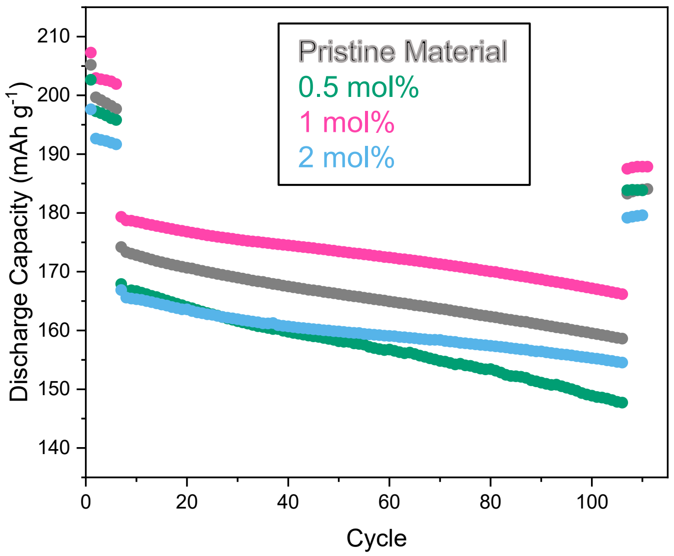
- Solution approach to create single crystal NMC particles, with controlled composition and surface coatings.
- Crystal control for suppressed micro-cracking, reduced voltage fade and increased cycle life.

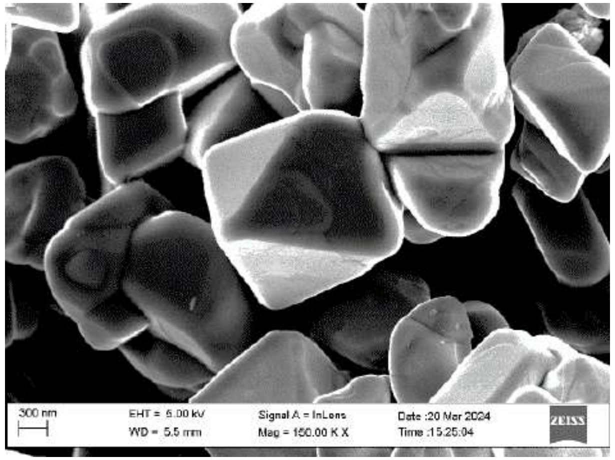
## Progress & Challenges

- High-capacity materials have been generated with impressive capacity retention. Initial tests suggest benefit for coatings with specific compositions and %s.
- Mechanistic understanding required for coating influence. Process optimization needed for direct recycling.




Energy Storage Materials, 2020, 27, 140-149



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# Modelling Activities

## Target & Motivation

***Modelling can be used as a guiding tool to optimise active materials,electrodes, electrolytes and overall cell designs.***

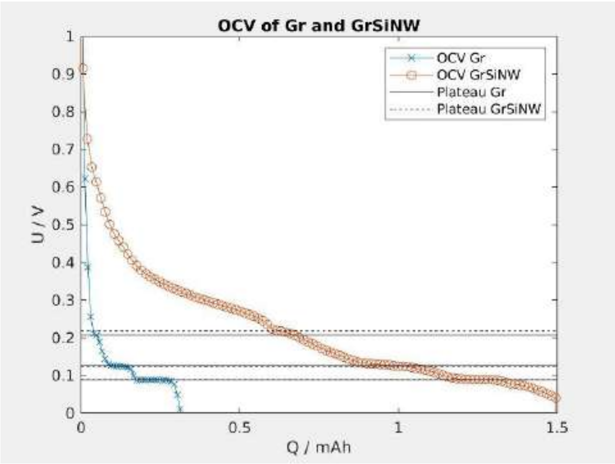
- Multifactor interrogation of the materials and cells can enhance the understanding of failure mechanisms.

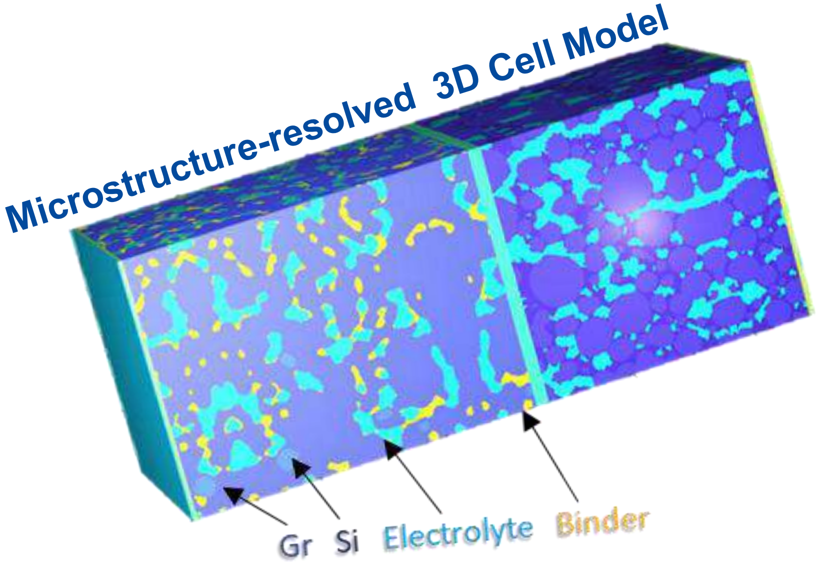
## Approach

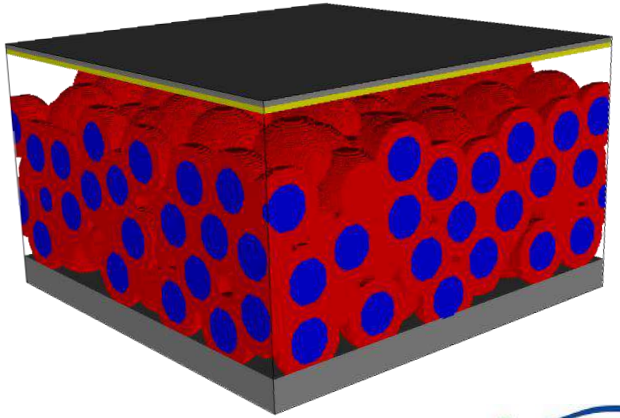
- Simulation tools based on a multiscale approach combining detailed models of materials and their interfaces in a homogenised 3D model on a cell scale (pseudo-4D models).

## Progress & Challenges

- OCV model of Gr and Si/Gr cell has been developed and will be used in further investigations.
- Electrolyte interactions with absorption on the NMC cathode surface.



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# Material Upscaling

## Target & Motivation

***Develop upscaling approaches for anode, cathode, electrolyte and separator, to allow full cell testing and ensure that the processes are scalable beyond the end of the project.***

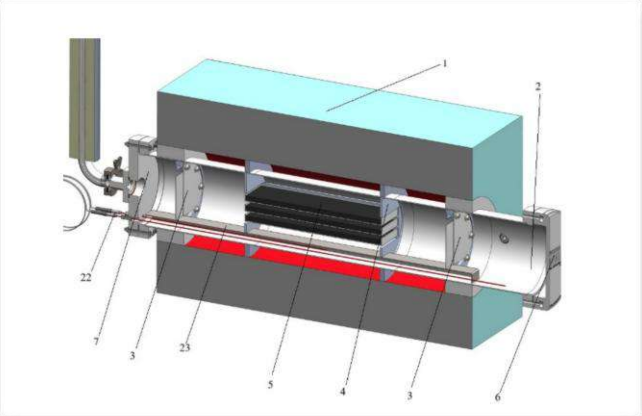
- Effective/green processing approaches needed at each step of the cell process (including recycling)

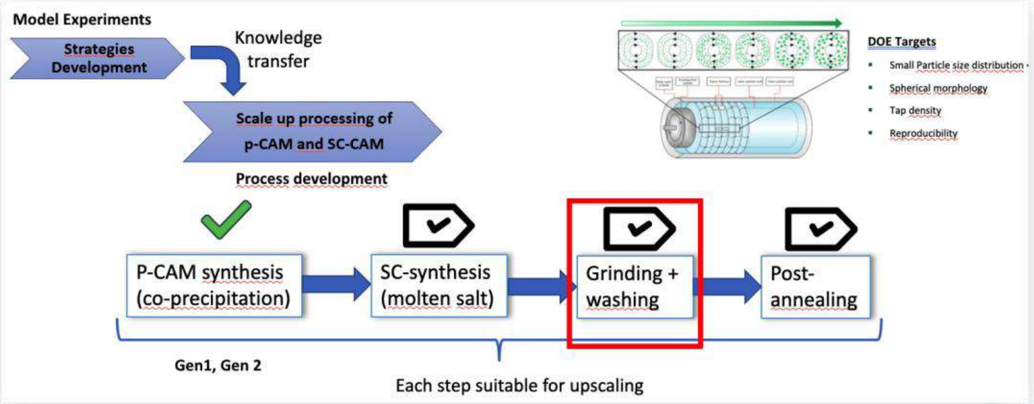
## Approach

- Anode-Prepare batch and continuous reactors to enable Si NW/Gr composite anode material formation
- Cathode-identify upscalable workflow for single crystal cathode formation

## Progress & Challenges

- Initial batch reactor for anodes has produced a range of Gens with different capacity. Some delays with obtaining parts for batch reactors.
- Some cathode conditions yield polycrystalline materials with lower cycling stability.



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# Full-Cell Testing, Recycling, BMS & Prototype Development

## Target & Motivation

***Combine optimised and scaled cell components for full-cell testing. Incorporate tailored BMS and test TRL6 prototype cells using relevant cell testing conditions informed by EV makers***

- Demonstration of SiGNE battery chemistry at TRL6 will allow for beyond SoA energy density demonstrations and suitability for EV applications to be illustrated

## Approach

- Cell testing at TRL 4 by **CID** using benchmark materials and partner materials.
- BMS system development by **ADI** and recycling process development by **TES.**

## Progress & Challenges

- Full-cell testing of different generation SiGNE materials is underway and is being benchmarked with commercial materials. Recycling of coin cells is being carried out, some delays in obtaining cells.


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# Key Output & Dissemination of SiGNE to Date

## • Scientific Publications

**ADVANCED MATERIALS**

Research Article | Open Access

**Fluorine-Free Lithium-Ion Capacitor with Enhanced Sustainability and Safety Based on Bio-Based γ-Valerolactone and Lithium Bis(Oxalato)Borate Electrolyte**

Khai Shin Teoh, Massimo Melchiorre, Sandesh Darlami Magar, Marius Hermesdorf, Desirée Leistenschneider, Martin Oschatz, Francesco Ruffo ... See all authors

First published: 22 January 2024 | https://doi.org/10.1002/adma.202310056 | Citations: 1

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**NANO · MICRO small**

Research Article | Open Access

**Understanding the Role of Imide-Based Salts and Borate-Based Additives for Safe and High-Performance Glyoxal-Based Electrolytes in Ni-Rich $NMC_{811}$ Cathodes for Li-Ion Batteries.**

Michel Klein, Markus Binder, Matjaž Koželj, Adriano Pierini, Tom Gouveia, Thomas Diemant, Annika Schür, Sergio Brutti, Enrico Bodo, Dominic Bresser, Juan Luis Gómez-Urbano, Andrea Balducci

First published: 10 June 2024 | https://doi.org/10.1002/smll.202401610 | VIEW METRICS

**ADVANCED ENERGY MATERIALS**

Research Article | Open Access

**Enabling Fluorine-Free Lithium-Ion Capacitors and Lithium-Ion Batteries for High-Temperature Applications by the Implementation of Lithium Bis(oxalato)Borate and Ethyl Isopropyl Sulfone as Electrolyte**

Fabian Alexander Kreth, Lukas Köps, Christian Leibing, Sandesh Darlami Magar, Marius Hermesdorf, Konstantin Schutjajew, Christof Neumann, Desirée Leistenschneider ... See all authors

First published: 25 February 2024 | https://doi.org/10.1002/aenm.202303909 | Citations: 3

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**InfoMat**

RESEARCH ARTICLE | Open Access

**Beneficial impact of lithium bis(oxalato)borate as electrolyte additive for high-voltage nickel-rich lithium-battery cathodes**

Fanglin Wu, Angelo Mullaliu, Thomas Diemant, Dominik Stepien, Tatjana N. Parac-Vogt, Jae-Kwang Kim, Dominic Bresser, Guk-Tae Kim, Stefano Passerini

First published: 28 June 2023 | https://doi.org/10.1002/inf2.12462 | Citations: 6

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## • Conferences and Other Presentations

- Cambridge EnerTech (CET)
- 39th Annual International Battery Seminar & Exhibit
- Gordon Research Conference (GRC)
- International Battery Materials Association (IBA)
- ICI
- Electrochemical Society (ECS)
- Dalhousie University
- Queens University Belfast, QUB
- ICACC2023
- XLIX- Physical Chemistry Division of the Società Chimica Italiana
- 74th Annual Meeting- International Society of Electrochemistry (ISE)
- IWES2024 -Third Italian workshop on energy storage
- 2nd Symposium for Young Chemists
- 9th EuChemS Chemistry Congress
- XXVIII National Congress of Società Chimica Italiana
- Transport Research Arena
- 75th Annual Meeting of the International Society of Electrochemistry (ISE)
- Swiss Battery Days 2024
- IBA2024
- 1st Young Chemists for Change

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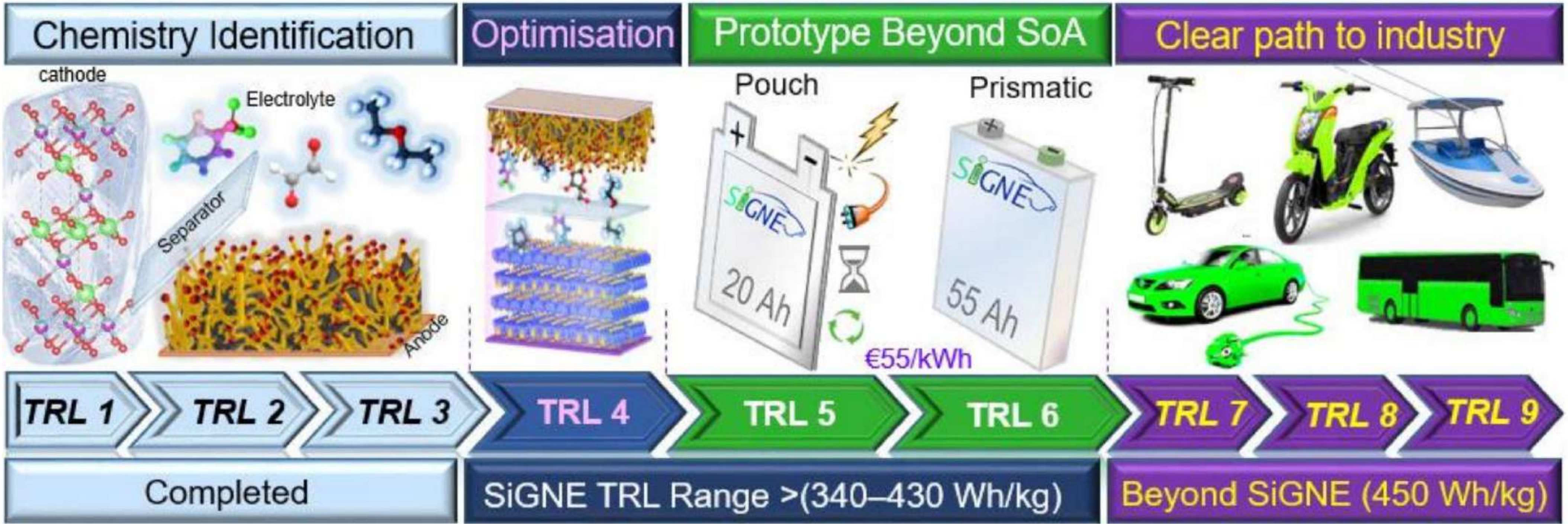
# TRL of SiGNE- Project and Beyond

- Progression approach from TRL 4 to TRL 6 and beyond by project end.
- Fabrication of small & large pouch 5-20 Ah and prismatic 55 Ah cell forms.

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SIGNE

# Contact Us

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