#H2020RTR21

MODALIS 2

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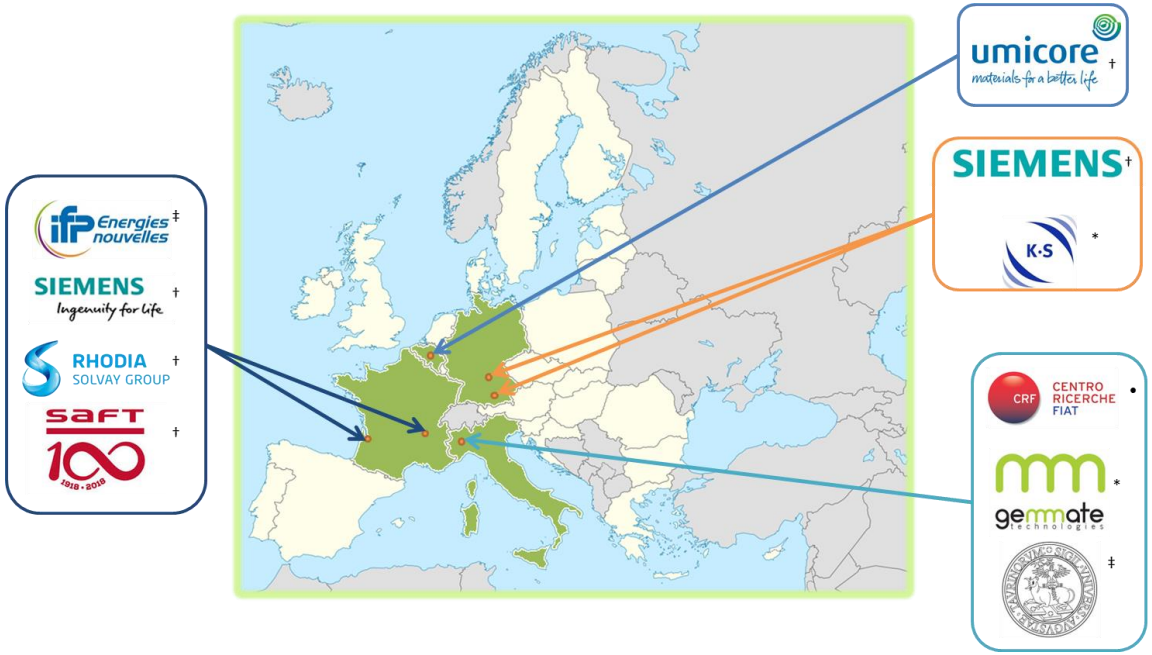
Overall project introduction

- **Call Identifier:** H2020 LC-BAT-06-2019
- **Budget:** €4,846,105
- **Start Time:** 1st January 2020
- **Duration:** 36 months
- **Topic:** Li-ion Cell Materials & Transport modelling
- **Types of action:** RIA Research and Innovation action
- **Coordinator:** IFPEN
- **10 partners**

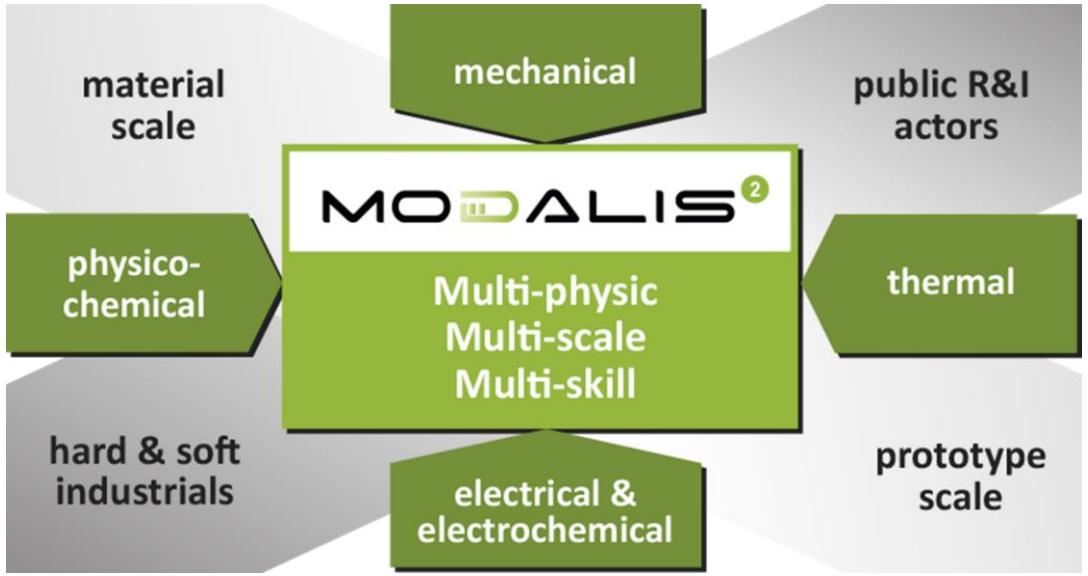


This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 875193.

Objectives of the project

- Development of a new simulation toolchain to provide stakeholders with necessary information:
  - Material manufacturers: material performances for future battery cells
  - Battery manufacturers: battery behavior based on material choices
  - OEM and end-users: integration of newly designed batteries in complete systems.

- Targeted on new and future technologies of Li batteries requiring new modelling
  - Gen 3b: Silicon based anodes
    - High volumetric expansion ➔ account for mechanical stress and deformation
  - Gen4: Solid-state electrolytes and Li metal for anode
    - Solid-state Li electrolytic conductivity
    - Li plating with Solid/solid interphase
    - Please limit this to 1 slide, and try to use quantified targets as much as possible



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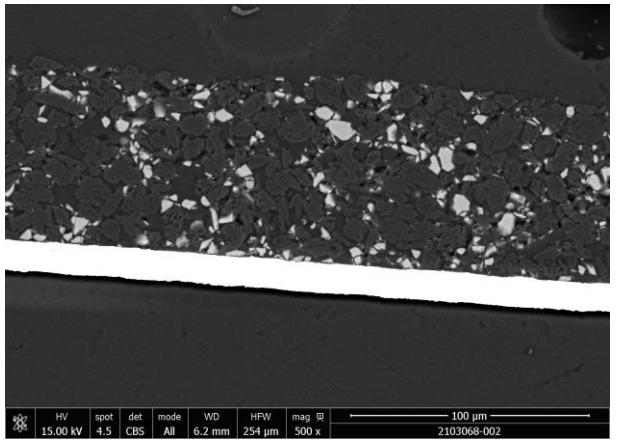
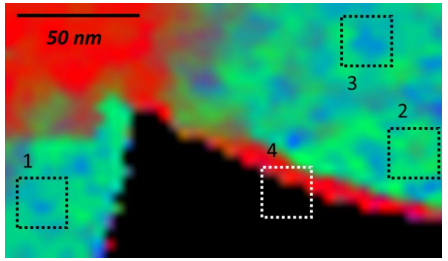
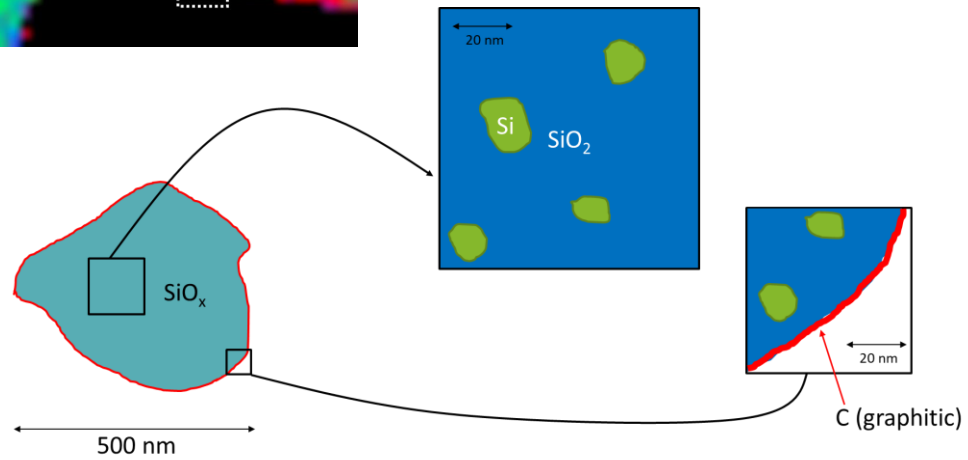
Production and characterization of Gen3b batteries material and electrodes

- Development of dedicated Gen3b cells for model validation
  - NMC811
  - SiOx/C with 20% Si
- Initial characterizations on electrodes
  - Understanding of negative material composition
  - Electrochemical characterization
  - Electrode swelling thanks to electrochemical dilatometry







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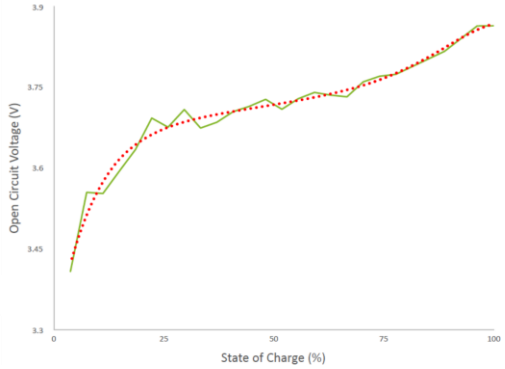
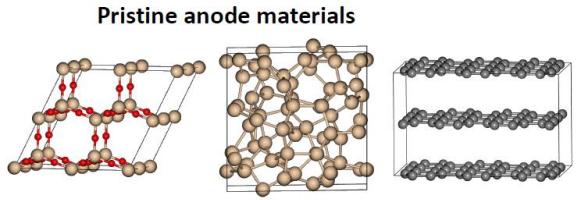
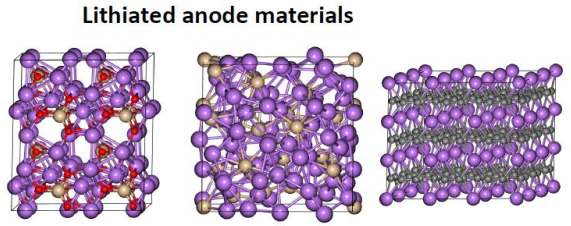
Atomistic and molecular modelling of Gen3b batteries

- Ab initio modelling to evaluate intrinsic properties of materials
  - Equilibrium potential of NMC material
  - Diffusion coefficients of NMC and Si based materials
  - Mechanical properties of Si based materials
- Can be used to evaluate continuum parameters of cell models from material development step







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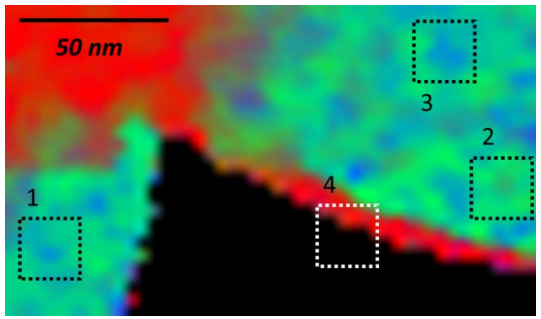
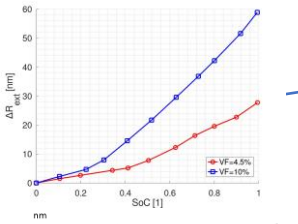
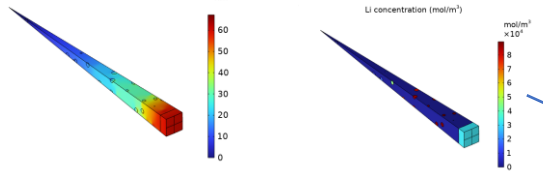
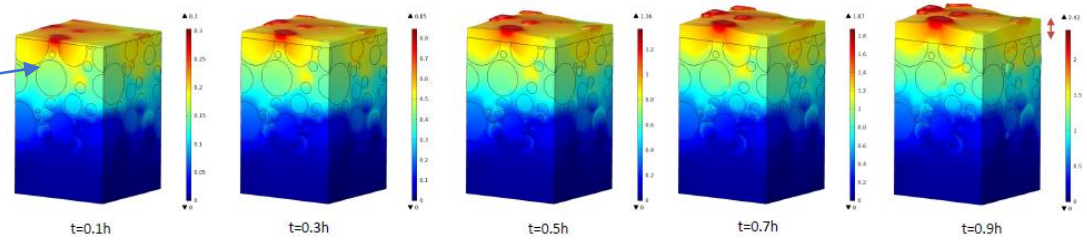
Microscale modelling of Gen3b electrodes

- Account for microstructure change on electrode behavior
  - Electrochemical impacts of electrode swelling

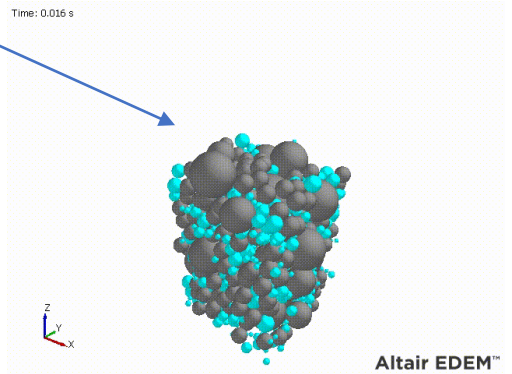


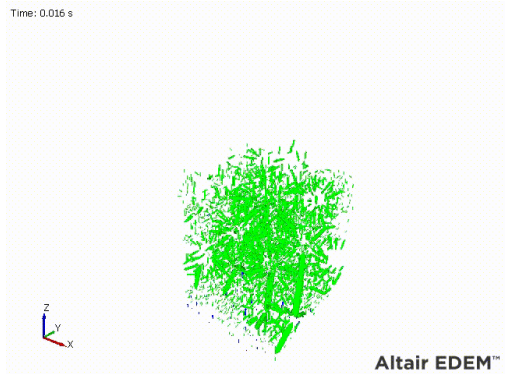






  - Mechanical effects
    - Electrode stiffness
    - Bond damage due to swelling





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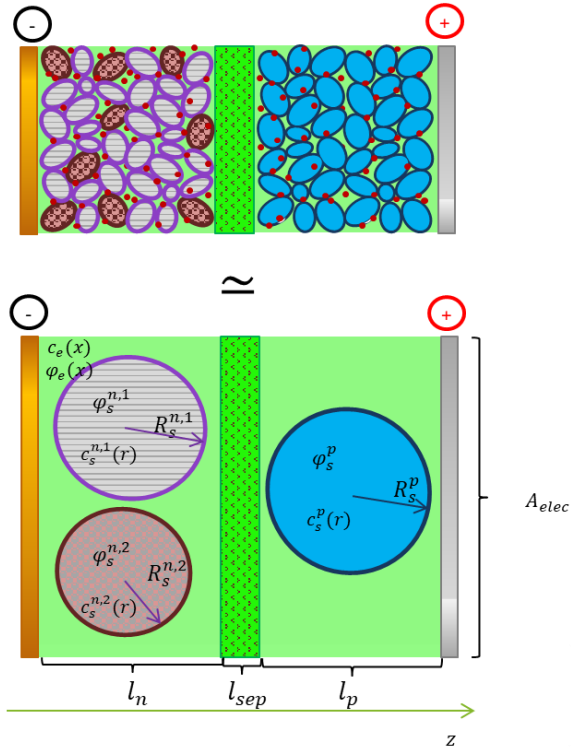
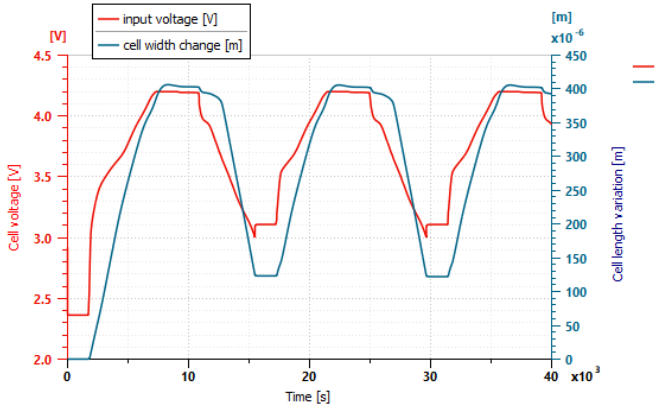
Continuum modelling of Gen3b batteries

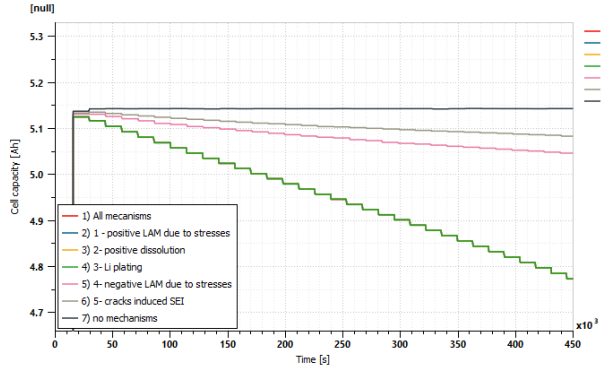
- Modelling dedicated to aging behavior
  - Fast computing SPM-e model with 2 materials in the negative
    - SiOx + Graphite
  - Mechanical behavior
    - Stress induced diffusion
  - Aging phenomena modelling
    - SEI layer formation
    - Li-plating
    - NMC oxidation
    - Mechanical effects
      - SEI cracking
      - LAM due to mechanical stresses



Cell voltage and swelling



Cell capacity fade upon cycling



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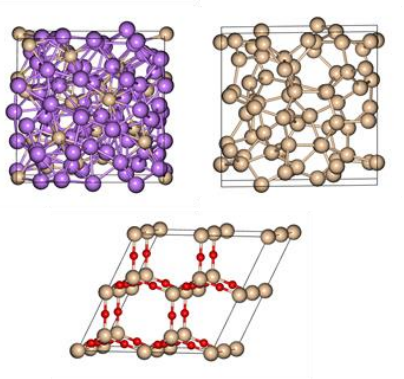
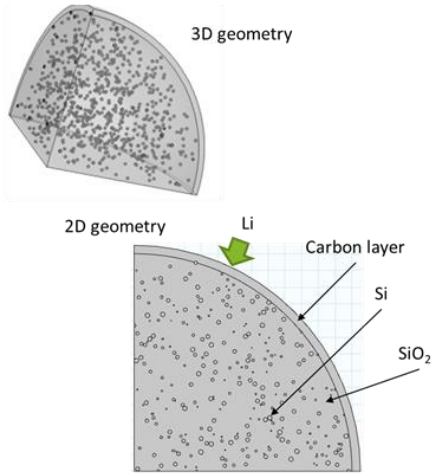
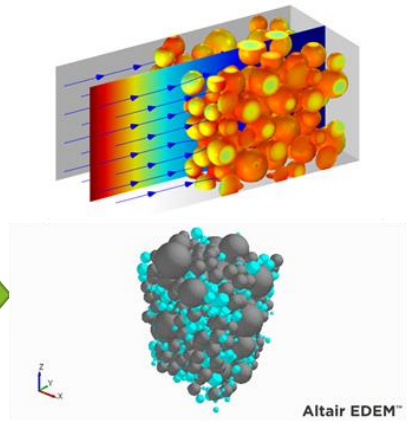
User oriented modelling toolchain



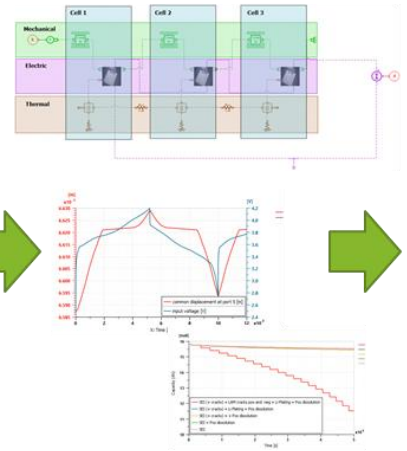
DFT modelling of lithiated Si and SiO_2



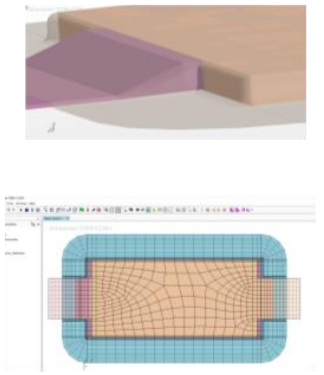
Mechanical behavior of Si/SiO_2 particles



Microstructure electrochemical and mechanical behavior



1D cell behavior



3D cell behavior

- Link of the several scales to create

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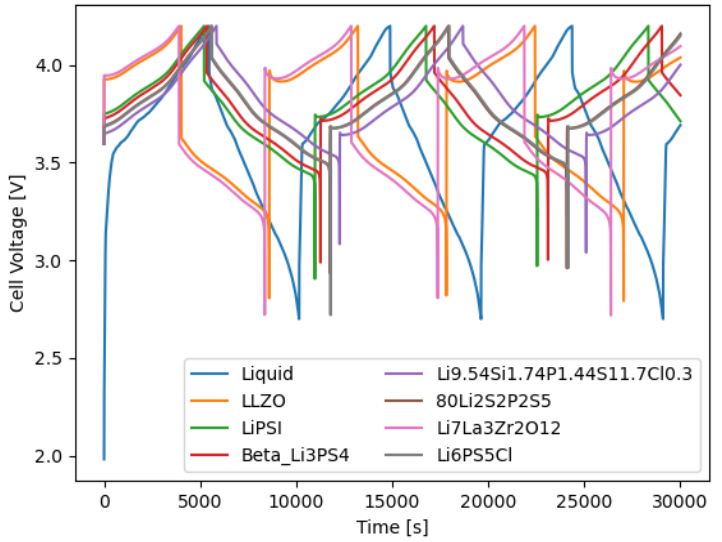
New modelling toolchain dedicated to solid state batteries

- Initial developments on Gen4 with sulfide electrolytes
  - Argyrodites with several formulations
  - Glassy sulfides
- Initial work on SPM-e model
  - Electrolyte model compatible with solid electrolyte
  - New development needed for Li/SE interface
- Atomistic / molecular modelling of solid-state electrolytes
  - Mechanical properties
  - Conductivities relying on former experience from Gen3b active materials
- Dedicated experimental work
  - Electrolyte conductivity
  - Dendrite formation



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Mid to long term expected impact of the project – Future industry needs

- Work dedicated on next generation batteries
  - Competitive advantage to EU industries by creating links between all stakeholders

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Mid to long term expected impact of the project

- Optimization of cell development all along the value chain
  - Use of a single toolchain for all stakeholders
    - Material manufacturers
    - Cell manufacturers
    - OEM
  - Better integration at all scale by accounting for relevant properties
    - Material properties
    - Design properties
    - Geometrical properties
- Development of new tools and knowledge dedicated to next generation batteries
  - Gen 3b with high Si content ➔ 2025
  - Gen 4 with solid electrolyte ➔ 2030

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Thank you

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