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MODALIS² PROJECT : DEVELOPMENT OF A MODELLING TOOLCHAIN FOR NEXT GENERATION BATTERIES

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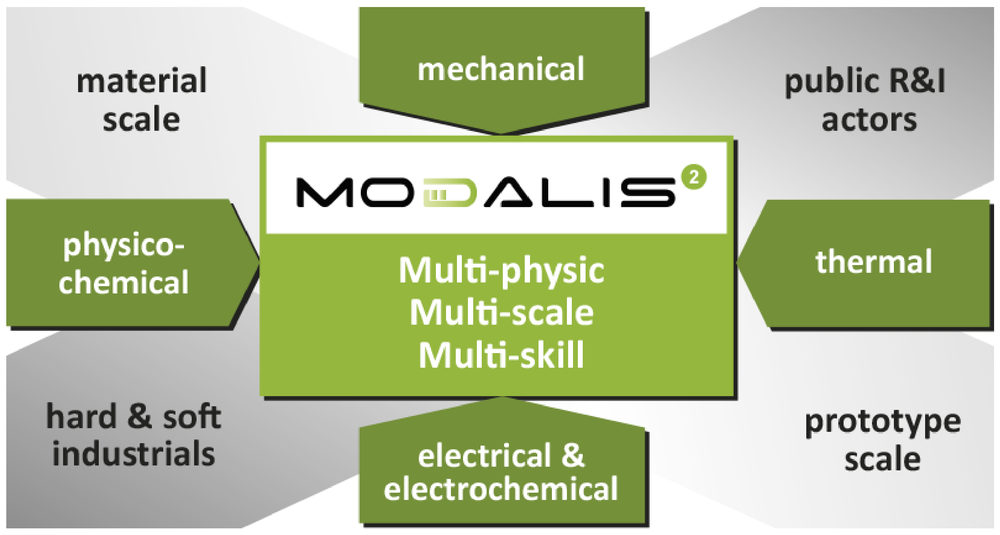
Introduction & Objectives

MODALIS² will provide degrees of freedom for the cell and battery development processes that allow to address the following design challenges:

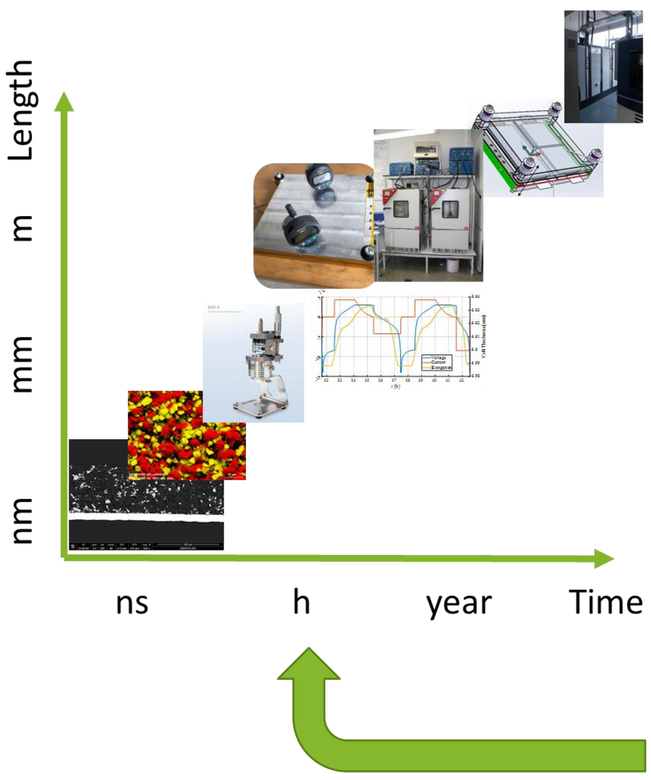
1. The need for faster development of batteries with higher energy density with new materials
2. The need for faster development of materials with higher optimized performances for higher-energy battery applications
3. Improved battery safety, both during transport and operation
4. Optimization of cyclability by using MODALIS² tools
5. Lower development costs
6. Better understanding of material interactions within the cell



2 targeted technologies

- ***Gen 3b: high performance cathode (NMC811) and anode (20 w% Si)***
  - Mechanical effects to be accounted for due to high volumetric expansion of the material
- ***Gen 4: Solid state electrolyte with Li metal***
  - Modelling of solid electrolyte transport behavior
  - Li plating to be modelled depending on solid electrolyte properties

Mutiphysics/Multiscale tool chain



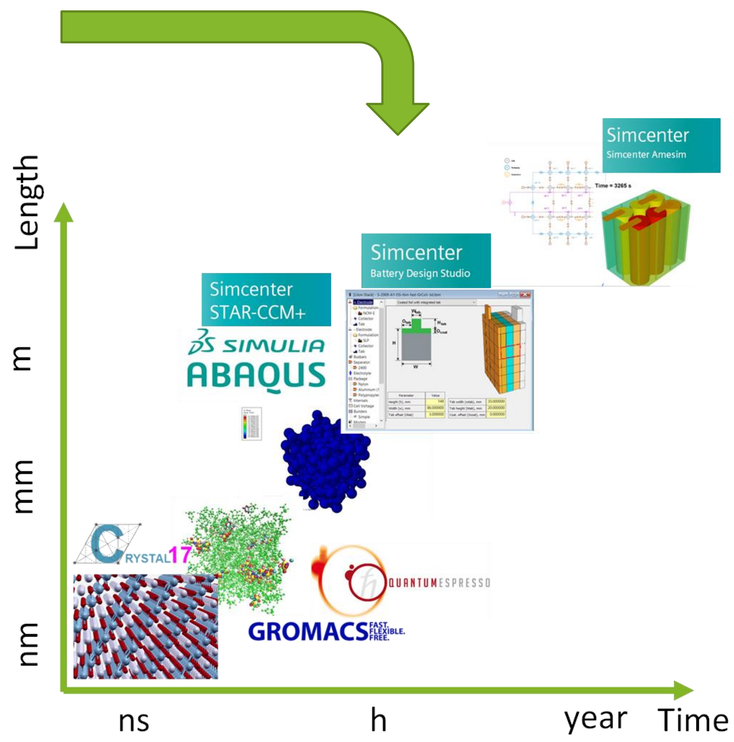
Multiple modelling tools available from material to cell

- Atomistic/molecular modelling
  - Intrinsic properties of the materials (transport, interfacial, thermal, mechanical properties)
- Microstructure modelling
  - Mostly dedicated to mechanical effects
- Full cell model
  - Evaluation of cell performances with aging and safety

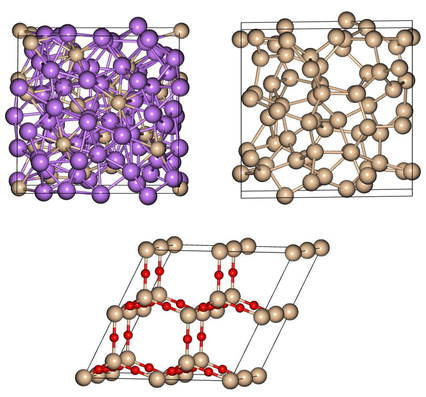
Need to create link in order to pass parameters and adapt model between scales

Dedicated multiscale experimental

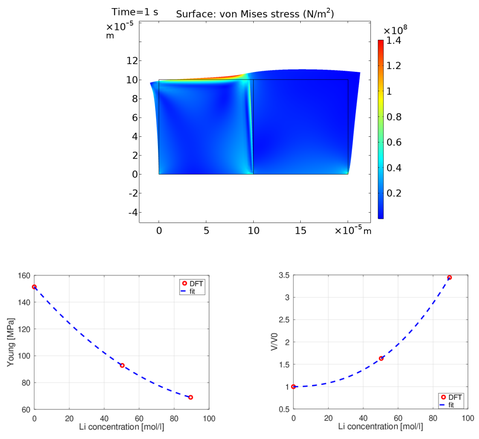
- Physical-chemical characterization
  - To assess microstructure of the electrodes
- Mechanical measurements
  - At electrode level
  - At cell level
- Aging campaign
  - With *post-mortem* analysis
- Safety tests



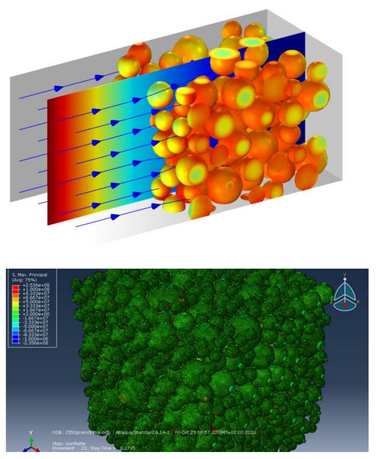
Application to Gen 3b cells mechanical behavior



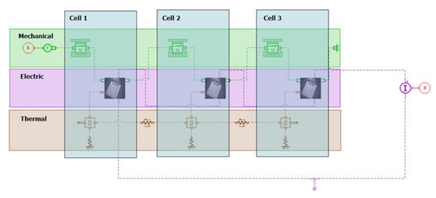
DFT modelling of lithiated Si and SiO_2



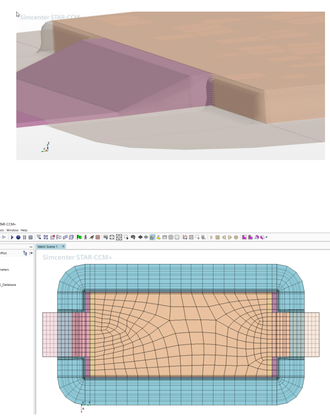
Mechanical behavior of Si/SiO_2 particles



Microstructure electrochemical and mechanical behavior



1D cell behavior



3D cell behavior

Conclusion and perspectives

On going development on Gen 3b

Tool chain developments implemented from atomistic to cell scale
Need of Gen 3b cells tests to validate the modelling approaches

Future developments on Gen 4

Choice of electrolytes of interest to be modelled (LLZO, Sulfide, Argyrodite)
Use of molecular modelling to assess electrolytic conduction
Development of a dedicated Li plating model for negative electrode interface stability modelling

Sensitivity analysis of model to be performed to estimate manufacturing uncertainties from material to cell