MODALIS 2

MODelling of Advanced LI Storage Systems

MODALIS²

A significant contribution to a cost-down for next generation EV battery cells

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In MODALIS², an innovative model-based multiscale and multi-physics toolchain will be set up to enhance and accelerate the development of next generation batteries (Gen3b and Gen4) and their materials. For that purpose, a multi-skills team forms the partnership of MODALIS² project to ensure the best cross-fertilisation.

Objectives

With the integrated modelling and simulation approach, will provide degrees of freedom for the cell and battery development processes that will then allow addressing 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

The main achievement and contribution of MODALIS² is therefore to develop and validate modelling and simulation tools for the following next generation batteries:

- **Gen 3b:** aiming for higher capacities for the positive and negative electrodes
- **Gen 4b:** enabling the use of solid electrolytes for improved safety and to facilitate the use of Li-M for the negative electrode

Multi-scale/Multiphysics approach

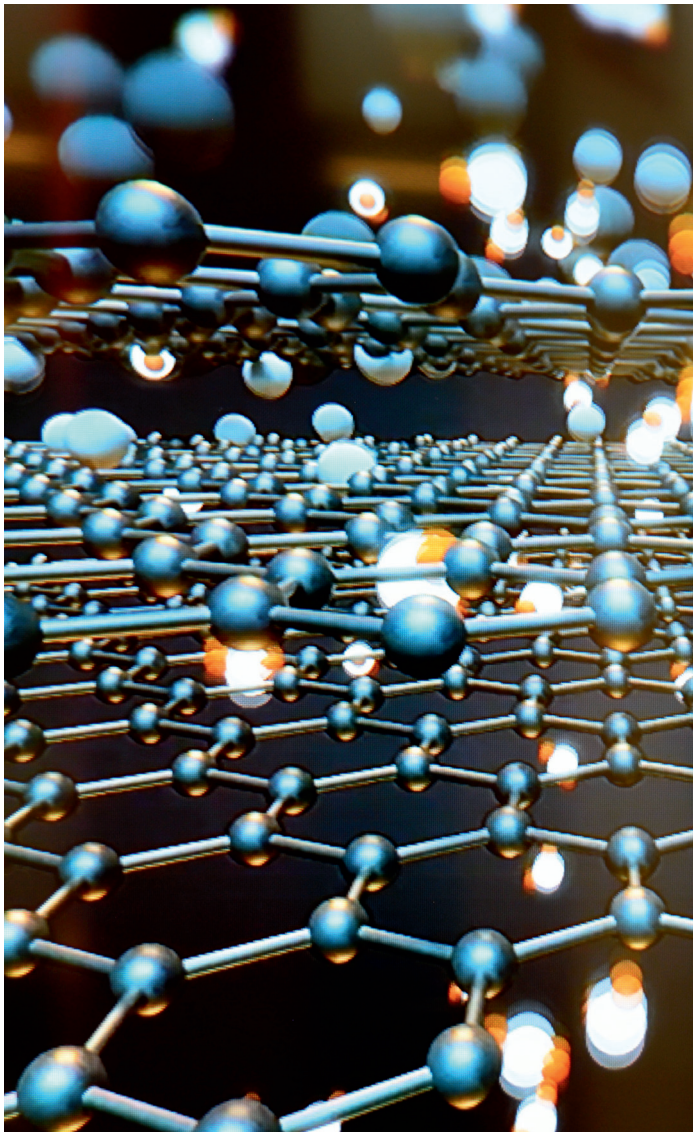
In new generations of Lithium batteries, the introduction of silicon (Gen3b) and solid electrolytes (Gen4) will deeply modify the inner behaviour of cells, since many interfaces and material components will be revisited. In that context, new skills are required to tackle the all extent of phenomena having an impact on the general behaviour of cells with solid electrolytes. There is an extended need of multi-physics approach coupling the following issues:

- **Electrochemical:** linked to the reversible transformation of electrical energy into chemical energy
- **Electrical:** describing electron transport into electrodes
- **Physical-chemical:** related to Lithium storage into crystal lattice, crystal lattice behaviour, Lithium transport in electrolytes…
- **Mechanical:** responsible of volumetric change of active materials, electrodes and cells as well as inter-faces degradations
- **Thermal:** coupled to above mentioned, governing the acceleration of transport phenomena, the electrochemical reaction kinetics and also the thermal runaway occurrence.

Multiscale modelling

The multiscale approach is necessary to tackle all new phenomena occurring in both Gen3b and Gen4b batteries. From molecular dynamics in ab initio modelling to cell/module behaviour through system modelling. Each phenomenon will be described at the relevant level (e.g. Interface behaviour at molecular level, thermal behaviour at cell level) to avoid unnecessary calculation burden and then implemented in higher level to assess the impact of specific mechanism at large scale (e.g.: mechanics behaviour and cell swelling at cell scale).

The Simulation toolchain approach is to develop a new continuous multi-physics, multi-scales and multi-skills suite of tools by upgrading, improving and couplings existing and validated tools for state of the art battery technologies. To do so, we'll rely on existing Siemens Simcenter tools, Battery Design Studio (BDS) and Amesim.

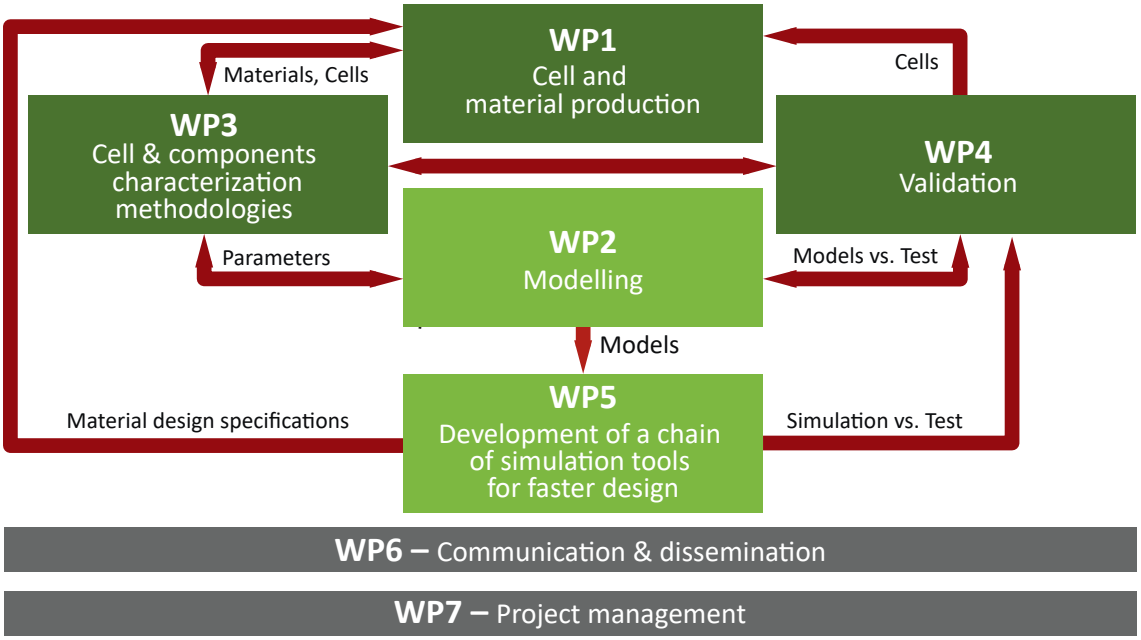


A round-table approach

The ambition of MODALIS² concerning interlinking all stakeholders related to cell and battery use and manufacturing is to initiate – together with other European-funded R&D projects in the area of battery and cell research and manufacturing – a continuing dialog about how to strengthen the European battery industry and reduce dependencies from outside-Europe suppliers. In this context, MODALIS² will in close cooperation with the European Commission and the other projects under the LC-BAT funding scheme work towards an industry-wide round-table on sustainable innovations in the cell and battery industry. The MODALIS² partners plan to host one such round-table and contribute to the agenda-setting in the industry with the research results produced by the project.

WP Structure

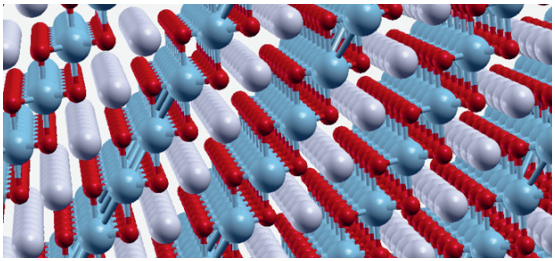
The MODALIS² project is implemented as an all-connected collaborative effort between the R&D work in WP1 through WP5. Center part takes the modelling in WP2, which uses data from the cell and component characterization performed in WP3, which in turn relies on inputs from the cell & material production in WP1. Models are then validated in WP4 and integrated in the simulation toolchain in WP5. However, there are several feedback loops, where e.g. the modelling in WP2 provides input to cell & component characterization methods developed in WP3 as well as the validation approaches developed in WP4. There are further feedback loops from the toolchain development in WP5 to WP1 concerning the cell & material production as well as WP4, where the validation also embraces the simulation tools.



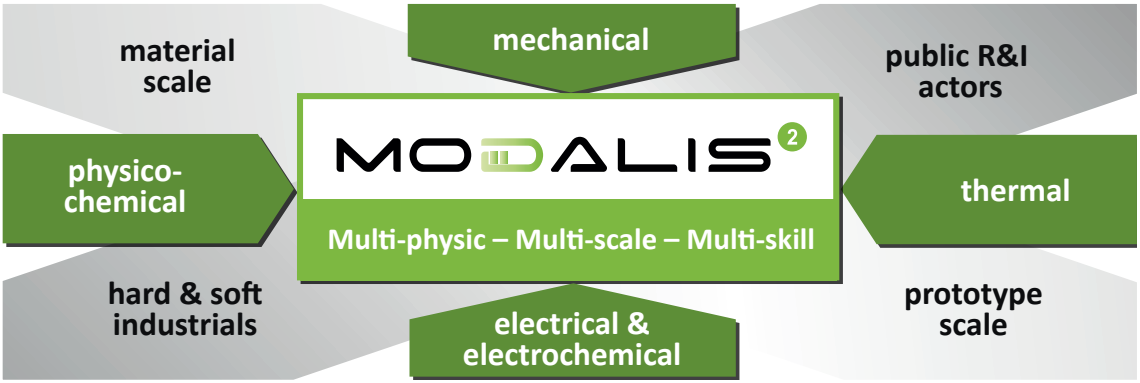
MODALIS² Consortium

All value chain for battery

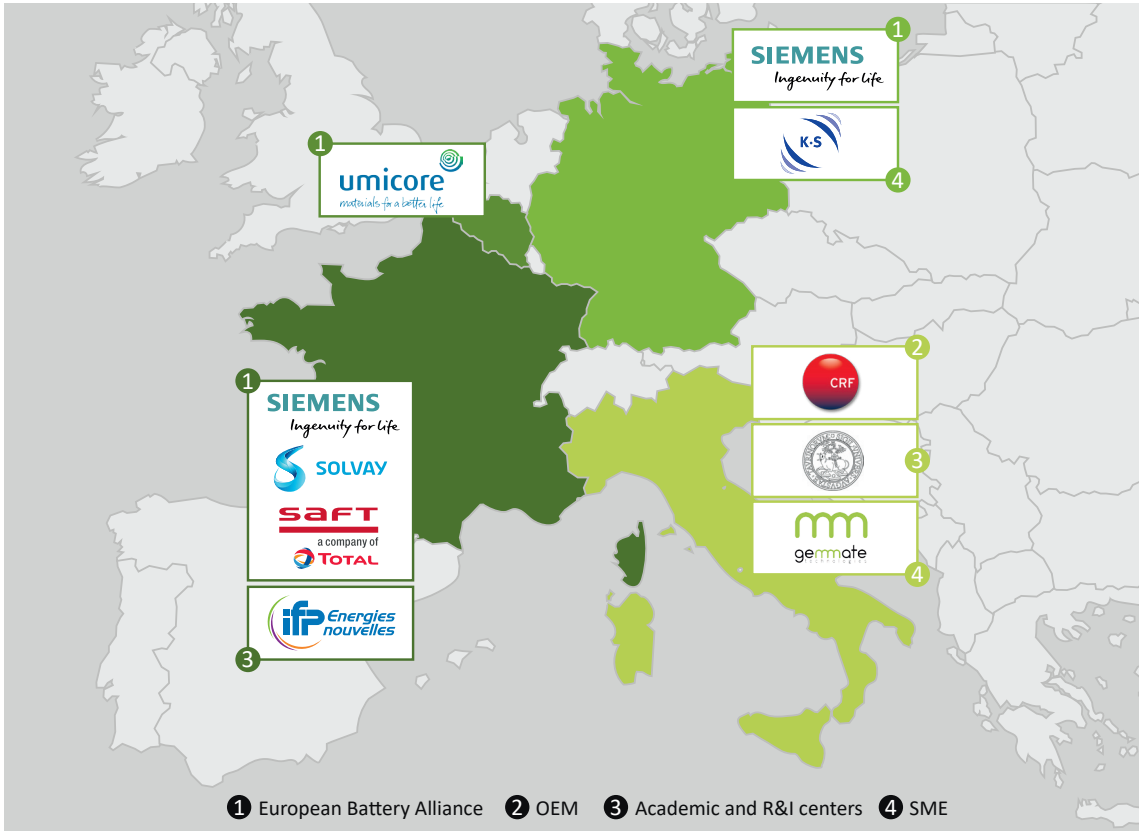
The consortium as a whole is well composed and positioned for tackling the modelling and characterization challenges. From academic to industry and comprising end-users, the project covers the entire value chain of battery developments from materials to integration. This will facilitate research and development progress beyond the state-of-the art and significant advances for both characterization and modelling and their direct application into commercial software (CRYSTAL, BDS, Amesim). Industrial partners will be able to guide tool and model development to cover their specific needs; these newly developed and integrated models and tools will be used right away by industrial end-users with different expectations.



- **Academics and R&I actors**
- **SME**
- **Industrial partners**



All skills needed for battery design and manufacturing



The consortium has been built on Europe's best capacities and expertise (industry and research) in the area of experimental characterization of materials, modelling and simulation from atoms to system as well as manufacturing of materials and cells for new-generation batteries.

www.modalis2-project.eu

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