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MODelling of Advanced LI Storage Systems

STAKEHOLDER REPORT ON OVERVIEW OF PROJECT RESULTS

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1 **Nature:** R = Report, P = Prototype, D = Demonstrator, O = Other

Dissemination level PU = Public
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1 Introduction

In this deliverable, a general assessment of the actions realised in MODALIS² project is performed by each work package leader as well as each partner. This will summarise the main achievements of the MODALIS² project as well as the challenges faced and the lessons learned for both technical and organisational point of views.

1.1 MODALIS² purpose and objectives

MODALIS² main objective is to provide degrees of freedom for the cell and battery development processes that will then allow addressing the following design challenges:

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

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

- Gen3b: aiming for higher capacities for the positive and negative electrodes. The new materials used in this technology are challenging in terms of modelling due to their high volumetric expansion which will require specific new development in order to account for this phenomenon at material and cell level. Specific care was taken to model the interfaces and their behaviour during volumetric expansion.
- Gen4b: enabling the use of solid electrolytes for improved safety and to facilitate the use of Li-M for the negative electrode. These solid electrolytes require new developments in order to account for the specific mechanisms responsible of solid-state ionic conductivity as well as the interfacial phenomena occurring in hybrid solid electrolytes and at the interface between active material and electrolyte.

MODALIS² added relevant effects for next Gen Lithium Ion batteries to state-of-the-art simulation tools. This enables the industry to incorporate new and innovative materials within their next generation Lithium Ion battery cells.

2 Work Package Report

The Work Packages (WP) are described in Figure 1.

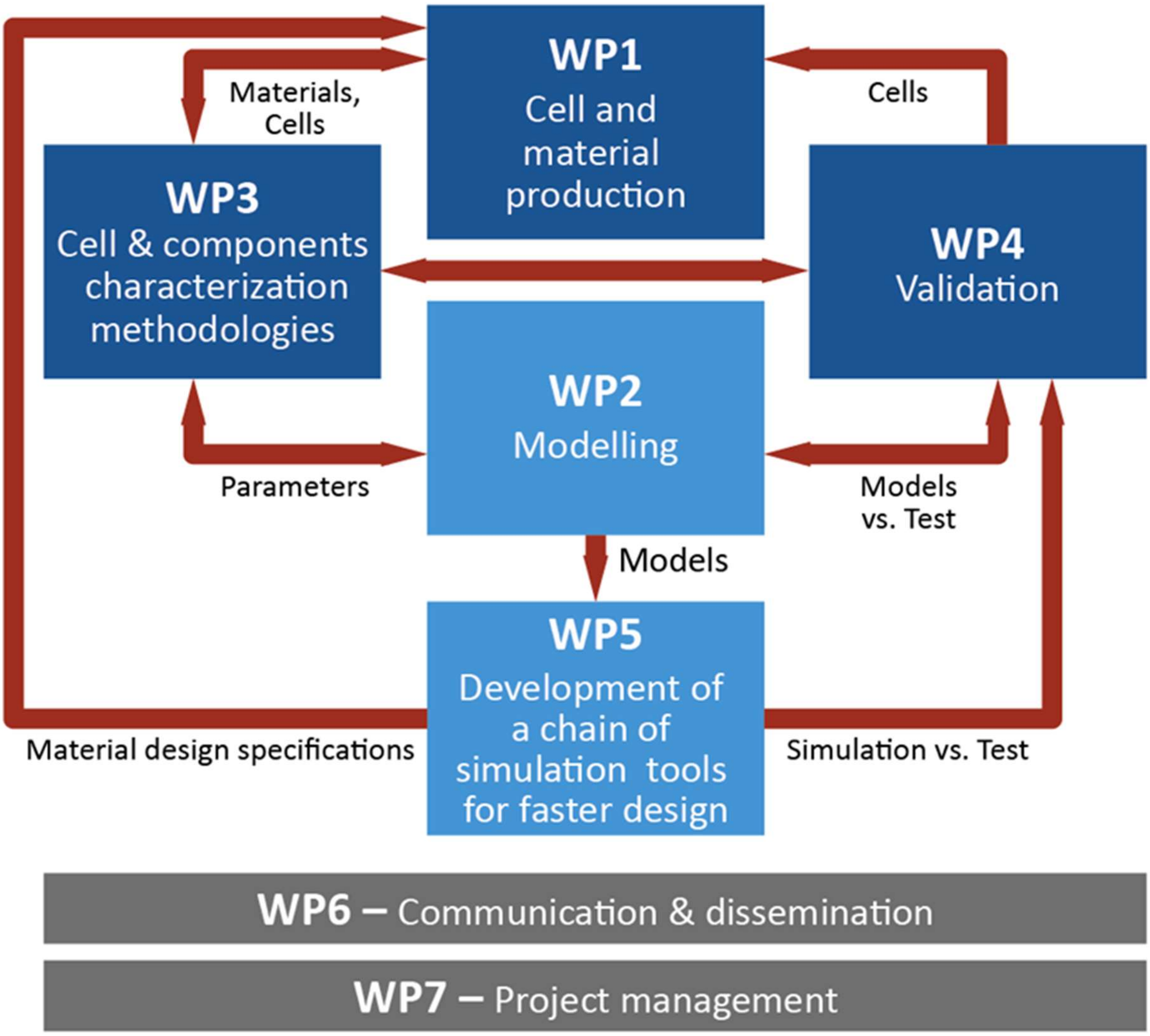

Figure 1: WP distribution

2.1 Work Package 1 – Cell and Material Production

The objective of this WP was to provide the MODALIS² project with material and cells. That was the input for experiments performed in WP3, model development in WP2 and model validation in WP4.

2.1.1 Achievements

Two cell generations were investigated in the MODALIS² project in order to focus on next battery generations.

Gen3b

- A positive NMC811 electrode material was provided by UMICORE to be integrated in the produced cells
- A SiOx/C negative material was purchased from an external supplier with 22w% of Si.
- First coin cells were produced and send to partners to check material performance once integrated in electrodes.
- Using initial numerical tools available from SISW, SAFT designed initial cells based on material properties
- 2 batches of 5Ah Gen3b cells were purchased using MODALIS² materials and sent to partners for characterisation

Gen4

- Fit for purpose material for Gen4 cells have been chosen by UMICORE, SAFT and SOLVAY.
  - Li/In foils for negative electrode
  - Argyrodite as solid electrolyte
  - NMC811 for positive electrode
- Li/In foils were prepared by SAFT for investigation and manufacturing procedures were shared among partners for further investigations in WP3
- 2 batches of electrolyte were manufactured by SOLVAY for integration into cells
  - Samples of electrolyte were provided to UNITO and IFPEN for further investigations
- 2 batches of cells were produced by SAFT and sent to project partners
- Positive electrode pellets were also produced and sent to IFPEN for further investigations in WP3

2.1.2 Challenges

Negative material had to be found at the beginning of the project. A first commercial material was purchased but after initial characterisation it came out that the silicon in it was not working. Consequently, another material was chosen with better performances.

Integrating >20%w of Si in negative electrode material is challenging as the material is still under development and leads to a high mechanical unstability.

Working on low TRL technologies leads to manufacturing difficulties and lack of robustness in the cells manufactured.

Labelling of Gen4 cells can raise safety issues at companies preventing them shipping the cells to other partners.

2.1.3 Lessons Learned

First steps in modelling projects should always consider a mature technology to ensure that initial steps are easy and allow a fast implementation of further tasks.

Mitigation measures are of utmost importance when considering cell manufacturing to ensure a positive outcome of the project and reduce risks.

2.2 Work Package 2 – Modelling

The WP2's objectives were to develop tools and submodels from atomistic level to full cell level partaining to specific phenomena occurring in Gen3b and Gen4b batteries.

2.2.1 Achievements

2.2.1.1 <u>Gen3b</u>

A multiscale multiphysics modelling approach has been developed and applied to account for mechanical behaviour of Li-ion batteries. As presented in Figure 2, multiphysics modelling was applied from atomistic level up until 3D cell level.

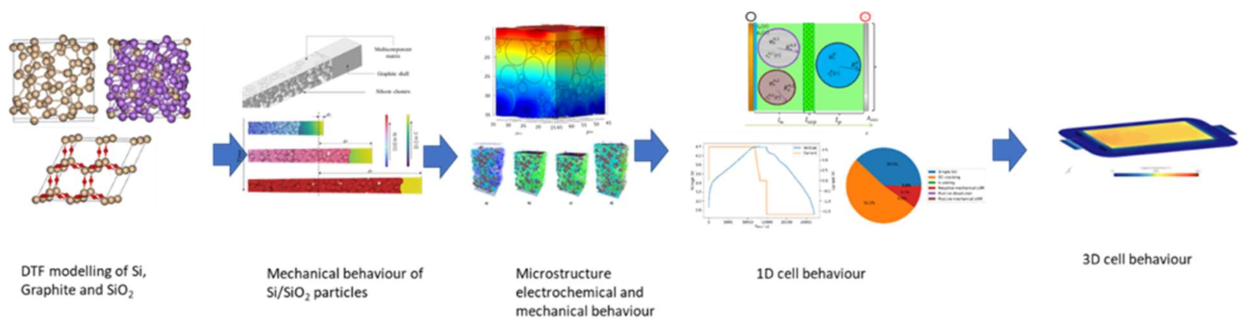

Figure 2: Multiscale modelling approach for Gen3b modelling

At atomistic level the modelling covered the following aspects:

- Transport properties of Li in NMC and Si based materials
  - Based on an initial approach applied to LNO and further applied to NMC investigations showed that diffusion coefficients obtained are in the same order of magnitude using several approaches and tools.
  - Depending on the assumptions made, the value of the diffusion coefficient can vary by several order of magnitude depending on the diffusion path chosen as well as the surroundings. This indicates that further investigations should be made to homogeneise the results at a higher length scale.
- Mechanical properties of Si based materials

- Several negative material were investigated to cover the one present in the negative MODALIS² material (Li_xC6, SiO_2, Li_2O, Li_4SiO_4, Li_xSi)
- Using DFT, volumetric expansion of each material was assessed finding especially the non-linearity of lithiated silicon swelling.
- Finally, the mechanical properties (Bulk, Young's and shear moduli as well as Poisson's ratio) of each phase of the negative materials were obtained using DFT. For lithiated silicon, the dependency of such properties as a function of state of lithiation was obtained.

Then the behaviour of the negative material was investigated at the particle level based on measurements on the material obtained in WP3. FEM approach was used to investigate the behaviour of negative material particles.

- Results from DFT modelling in molecular modelling were used as inputs for chemical and mechanical material properties. Several assumptions were made to investigate the impact of SiOx convertion into active or inactive materials
- Maximum Li concentration was determined based on these asumptions. The higher the conversion in cycling materials, such as pure Si, the higher the maximum Li concentration.
- Particle swelling was assessed based on the same assumption showing global particle swelling from 50% with no SiOx convertsion up to 150% with a full SiOx conversion.
- Transport properties parameters (such as the Bruggeman coefficients) were also investigated to assess their variation with the particles state of charge.

The swelling behaviour was then further used in electrode scale modelling with two approaches chosen.

- Non coupled mechanical modelling approach based on Discrete Element Modelling (DEM)
  - The apporach investigated the link between particle swelling and binder properties on electrode swelling behaviour. The output parameters investigated are the electrode density and thickness, bonds damage.
  - The simulation showed that the binder properties do not impact the overall electrode swelling behaviour as it is not stiff enough to prevent the electrode from swelling.
  - The external properties, such as applied pressure, as well as the binder properties, such as its strength, will impact the mechanical stability of the electrode as a too high external applied pressure as well as a weak binder will lead to high bond damage.
- A coupled electrochemical/mechanical modelling was performed.
  - An initial geometry was created thanks to DEM to place Si based and graphite particles according to experimental material properties. Then a representative volume of the electrode was modelled in FEM.

- Afterwards a 3D FEM modelling of the microstructure was performed showing the state of lithiation of the particles depending on their composition and their place in the electorde, the overall displacement of particles and electrode boundary and finally the stresses generated in the electrode due to swelling.

Finally, these results were further applied in 1D simulation to account for both electrochemical, mechanical and ageing behaviour.

- A SPM-e modelling approach acocunting for blend materials in negative electrode was chosen and main ageing mechanisms have been implemented into this model: SEI formation, dissolution of positive active material leading to positive active material losses and Li plating at the negative.
- Mechanically induced phenomena have been integrated in the model
  - Stress induced fdiffusion
  - SEI cracking
  - Loss of active matertial due to mechanical stresses
- A cell-swelling model has been implemented calculating the material volume variation and its impact at the cell level.

In parallel, a thermal runaway model has been calibrated and coupled to a electric equivalent circuit (EEC) of the battery.

2.2.1.2 Gen4

A similar multiscale/multiphysics approach was also developed for Gen4 batteries.

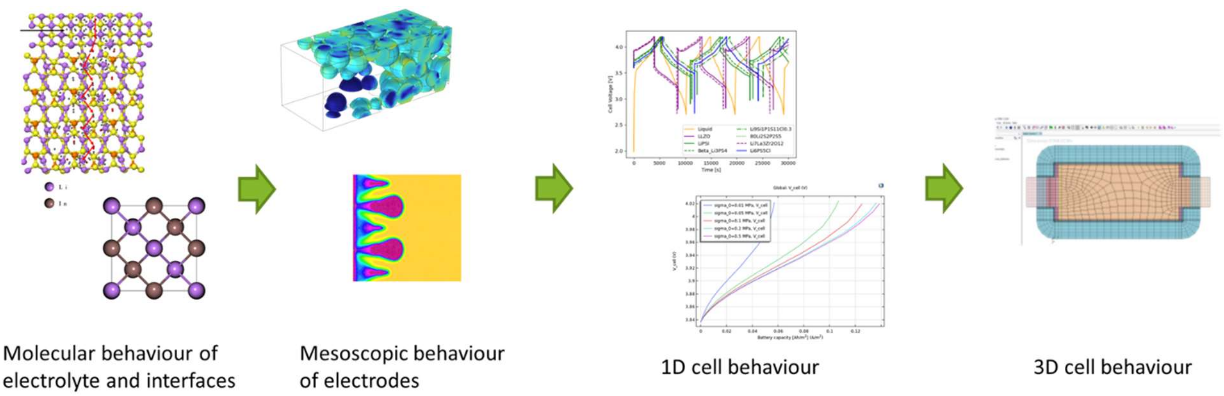

Figure 3: Multiscale and multiphysics modelling of Gen4 cells

At molecular level, the properties of argyrodite and interfaces with Li, Li/In and NMC were investigated, which showed:

- Li and Li/In exhibits several stable facets in agreement with the recent litterature validating the calculation approach
- The formation of a passivation Li2S layer at the negative electorde allowing the ASSB to work as the structures formed are electronically insulating but ionically conductive.

At the microstructure level, as for Gen3b two approaches were performed.

- The first one was dedicated to studying the stability of the negative electrode interface by performing a phase-field modelling approach. This approach assesses the dendritic growth of Li inside the solide electrolyte during charge.
- The second one is a 3D resolved mechanical/electrochemical model of the Gen4 battery showing the impact of cell assembly on battery behaviour and performance. Design parameters can be adjusted in order to assess their impact on cell behaviour. Finally, the swelling of the cell was also assessed in these calculations.

Finally full cell behaviour was also investigated by adding specific phenomena in a 1D battery model.

- The electrolyte has been modelled with single Li+ ion conduction and presence of negative vacancies as described in the litterature but applied to a mixed bulk battery at the positive and film electrode at the negative.
- The effect of external pressure has been taken into account by adding a contact law on the charge transfer kinetics.

2.2.2 Challenges

- DFT modelling of more advanced NMC material (with high Ni content such as NMC811 and higher) is challenging due to the size of the representative unit cell needed and the large number of configurations possible for such structures.
- Mechanical FEM simulation is not possible with very high deformations induced by Si material (300% assumed swelling). Other modelling approaches were investigated.
- 3D modelling at the electrode scale shows strong solving issue which requires model simplification.

2.2.3 Lessons Learned

Eventhough each scale modelling methodology is well known (but can still be improved) with existing tools and methodologies defined, upscaling from atomistic to mesoscopic to full scale modelligng is not straight forward - especially regarding complex microstructure where material properties are stongly anisotropic. Consequently, further developement regarding homogeneisation of diffusion properties is needed to account for primary and secondary particles of NMC materials.

Particle composition plays a role on mechanical behavior. Therefore, a particle scale modelling is necessary in order to understand the behaviour of particles before the integration in electrode scale modelling and further full cell modelling.

Due to the great technology's heterogeneity in gen4 as well as the low TRL of this technology, getting a generic and validated modelling approach seems still out of reach.

2.3 Work Package 3 - Cell & Components Characterization Methodologies

2.3.1 Achievements

At material scale, characterizations of Gen3b material and Gen4 electrolyte have been performed as planned and showed reliable and repeatable results. This activity has provided all expected input for the other workpackages (WP2, WP4 and WP5), in compliance with the project objectives. It needs to be highlited that for Gen4, conductivity chacracterization versus temperature, investigation of pressure dependancy and dendritc growth study are valuable data for the understanding and the developement of this new technology.

Cell test plans have been defined for both Gen3b and Gen4 cells. These test plans were well optimised to provide enough data for modelling activity in WP2 using the smallest quantity of cells to be produced in WP1. The test plans have allowed to evaluate the cell initial performance and its behaviour under cycling as well as under calendar ageing. For Gen3b, abuse behaviour was also covered by the test plan. Furthermore, the test plan had sucessfully taken into account specificity of each new technology, i.e. swelling monitoring for Gen3b cell with dilatometer set-up and safety consideration according to safety restriction & handling conditions for Gen4 Sulfide cell.

All tests defined for Gen3b and Gen4 cells have been performed. Some key achievements in this part can be highlighted:

- Gen3b: Good repeatability was found from result between different batch and between partners.
- Gen3b: Post mortem analysis performed after ageing test showing ageing mechanism on anode side is the key contributor.
- Gen3b: Cell swelling over cycling sucessfully experimented using dilatometer. Correlation between cell sweeling and its state of health was demonstrated with experiment data.
- Gen4: Despite low TRL leading to higher discrepancy on characterization results than Gen3b, performance improvement was demontrated for the second batch thanks to some lessons learned (cell preparation and testing activity) from the first batch.

2.3.2 Challenges

One of the challenges identified from the beginning of the project was the test plan construction for new technologies. The test plan has to be a perfect compromise between enough data for modelling activity in WP2 and a reasonable number of cells to be produced in WP1. Furthermore, the test plan definition has to consider also specificity of each new technology, i.e. swelling monitoring for Gen3b cell with dilatometer set-up and set-up considering safety restriction & handling conditions for Gen4 Sulfide cell.

Due to difficulties to produce cells in WP1 a challenging plan shift had to be carried out within WP3. Hence, a redefinition of the test plan was performed with partners between WP1, 2 and 3 in order to be able to optimise the test plan using the lowest quantity of cells. This decision has helped to recover the overall planning of the project.

From the technical perspective, the Gen4 characterisation was a challenging task. Due to low TRL of the technology, the repeatability is lower than Gen3b and root cause analysis to understand low performance or discrepancy was very complex. Although the Gen4 results' low consistancy does not allow MODALIS² project to perform D4.5, the results from the second batch showed better performance of the cell and more repeatability inside the batch and also between partners' tests.

Finally yet importantly, to ensure safety despite new technologies involving new hazards and constraints was one of the major challenges. All partners in WP3 have rigorously respected the cell handling instructions and cell safety limits during experimentation. Consequently, any safety incident during the MODALIS² project was excluded.

2.3.3 Lessons Learned

The delivery and regular reminders of instructions on cell safety limits and cell handling conditions is mandatory to help the partners to work safely, especially with prototype cells.

The anticipation of test set-up for new technology is important to avoid losing resources and time. Indeed, at the time of the first Gen4 batch delivery, due to lack of test set-up for Sulfides at some partners' facilities, tests were performed several weeks after the cell reception. It led to the cells degradation (self-discharge) in the meantime and consequently to a lower performance than expected; however, the second batch cells have been tested immediately after reception and have demonstrated better performance and repeatability than the first batch.

2.4 Work Package 4 – Validation

As reported in the Grant Agreement, the WP4 objectives are here summarised:

- To define the expected validity domains of the models;
- To define relevant testing protocols that will be carried out experimentally (WP3) to validate the models;
- To validate the developed simulation tools by comparing experimental (WP3) and modelling (WP2-5) results.

After the validation the model will be used for several purposes:

- Producing a demonstrator relevant for the iterative process of Gen4b battery development whose results will be used in WP1
- Conducting a sensitivity analysis in order to assess the most relevant material/cell design parameters to be measured (WP3)

2.4.1 Achievements

During WP4 activities several achievements were reached:

- The KPIs for the validation of the toolchain developed by the MODALIS² project were identified. In particular, the end user needs and the requirements for the computational tools and methodologies for their validation were defined. The MODALIS² toolchain is composed by several codes:
- For electronic structure codes: Quantum ESPRESSO and Crystal
- For atomistic code: Gromacs and COMSOL
- For electrochemical continuum scale: Simcenter STAR-CCM+ and Simcenter Amesim

Thanks to this toolchain it was possible to generate the required data by STAR-CCM+ through the electronic structure and atomistic codes, simulate the cell behavior during cycling and the ageing phenomena that affects the cell.

- The models were validated for all the simulation scales:
- Electronic structure: the Quantum ESPRESSO and Crystal code results were compared in order to assure that the two codes produce coherent results. Acceptance criteria for the electronic structure calculations were fixed.
- Atomistic/mesoscale: a comparison between standard codes used today and software proposed by partners was performed. The validation of the benchmarked solutions was done following different parameters on different scales: molecular prediction including Li transport properties, charge-discharge prediction for the cell behavior simulation during cycling.
- Continuum: this validation was performed by comparing cell scale experimentation with STAR-CCM+ and Simcenter Amesim calculation. The voltage, current, temperature and swelling profiles were replicated including duty profiles close to realistic operating conditions (WLTP).
- Case studies were defined and the related simulators were produced. Depending on the complexity and the nature of the case study different simulators were produced with Simcenter Amesim or STAR-CCM+.
- Key material characteristics to efficiently define and design a virtual model for Gen4 were defined. Characteristic were detailed for positive electrode, solid electrolyte and lithium anode.

2.4.2 Challenges

Different challenges were faced during the MODALIS² project duration:

- The COVID-19 world-wide pandemic situation influenced the cell production and, consequently, the testing and production of experimental results needed for the validation of the simulation tool.
- The Gen4 cell production faced several issues. For this reason only a few experimental results were produced. Moreover, the Gen4 testing was preformed nearly at the end of the project and it wasn’t possible to build and validate simulators based on experimental results.

- Delays were faced for the software installation at different partners' site (STAR-CCM+ and Simcenter Amesim).

Monthly calls were organised between WP4 partners in order to monitor the progresses, to evaluate the delays and apply counter measures to mitigate them.

2.4.3 Lessons Learned

Thanks to the WP4 activities, new skills and knowledge were developed and shared between all the partners involved: definition of the key cell characteristics to monitor the simulators development, gained experience with the simulation tools to autonomously model the simulators of interest.

2.5 Work Package 5 – Development of a Chain of Simulation Tools for faster Design

In order to facilitate the understanding of the WP5 achievements, a recapitulation of workpackage 5 objectives is presented below:

The goal of the Workpackage 5 was to achieve the required progress in the field of battery dynamic simulation, from battery technology range supported, to improved prediction and multi-scale representativeness. Moreover, the new toolchain will mandatory support the models from workpackage 2.

More specifically, reaching the goal requires the following achievements in this workpackage:

- improvement of Simcenter Battery Design Studio (BDS) (which was replaced by Simcenter STAR-CCM+ as more appropriate to integrate the model development) and Simcenter Amesim (Amesim) to address specific behaviour of Gen3b and Gen4 technologies
- supporting models from WP2: 3D macro homogeneous Cell level model, 3D electro-thermal models, 1D models or neural networks.
- continuous interoperability of models from the different scales (3D/1D) and tools realising the simulation toolchain
- fast model transfer techniques from 3D to 1D, as possible using standard interfaces like FMI
- functional demonstrators prototypes to be used in WP4 to generate numerical demonstrators to showcase the capability of the new models.

2.5.1 Achievements

WP5 efforts were focused on the following three main tasks in order to achieve the above mentioned goals:

- Implementation work

  - Improvement of Simcenter STAR-CCM+ (STAR) and Simcenter Amesim (Amesim) to address specific behaviour of Gen3b and Gen4 technologies
  - Supporting models from WP2: 3D macro homogeneous Cell level model, 3D electro-thermal models, 1D models or neural networks.
  - This objective has been partially achieved with the full completion of the model integration supporting the simulation prediction of Gen3b cells in both STAR and Amesim, only Gen4 model derivation and implementation is incomplete.

- The Gen3b model has been implemented by IFPEN in Simcenter Amesim as a specific new component in the Electirc Storage library. It will be industrialised in a future version of Amesim, making it available for our customers in the course of 2024.
- The Gen3b model implementation has been completed and integrated into the official Simcenter STAR-CCM+ release codes. This means they will be available for downloads to our customers' base in the course of 2024.

  Initial results were presented at the NordBatt Conference in 2022. Finally, demonstrators have been parametrised to be used in validation of the implementation work and are used by contributors of WP4
- The implementation of Gen4 models in both STAR and Amesim is incomplete and may not be achieved by the end of the funding period due to several factors:
- The pandemic situation at the beginning of the project delayed a lot of activities
- Technical challenges in deriving models from the analysis of experimental Gen4 cells.

However, it has been decided to work on a smaller, yet comprehensive approach, which is more like a methodology rather than a code implementation and this will be delivered as a demonstrator for the end of the project

- Continuous interoperability
- Model transfer from the different scales (3D/1D) and tools realizing the simulation toolchain
- Fast model transfer techniques from 3D to 1D, as possible using standard interfaces like FMI
  WP5 worked on the parameters transfer at various scales. It ensured identical model parameters inputs between 3D and 1D to support ease of workflow for scale interfacing and providing numerical consistency to ensure error-free setup and easy interpretation of data inputs at both scales (3D and 1D). Initial investigations on the use of a standardised file format for parameter exchange (BPX format, https://bpxstandard.com) have been done, and python scripting for Amesim has been investigated. The parameterisation of equivalent circuit models from the SPM-e Gen3b model.
- Functional demonstrator prototypes to be used in WP4 to generate numerical demonstrators to showcase the capability of the new models.

- This work is still in progress with Amesim and STAR, but demonstrator simulations are already in place and leveraging the implementation achievement mentioned above. These demonstrators contain the most up to date model with respect to the progress of the overall project, meaning the Gen4 cell demonstrator are not part. Only the Gen3b cell demonstrator has been parametrised

2.5.2 Challenges

There has been quite some challenges throughout the project but we were well supported by the project coordinator to address them or to find an appropriate solution

- Siemens required an agreement amendment to allow for the integration of additional resources into the project coming from Siemens German subsidiary
- The process took some time, mainly with respect to the hiring process
- This was completed successfully as the additional resources from Germany could join the project and contribute significantly to D5.2 and D5.3
- The COVID-19 world-wide pandemic situation also caused some challenges to recruit the appropriate personnel to address the work in workpackage 5.
- This led to some delays as to engage the hiring process
- This was a constraint which wasn't under our control
- Delivery of the derived models from research effort (experimental or modelling) has high impact on the implementation completion. Any delay to the model delivery is a direct consequence on delay for model implementation
- The monthly calls put in place between WP2 and WP5 helped getting a clear visibility in the model derivation and model implementation progress
- This allowed to adjust and compromise on the priorities and the approaches taken in the objective to achieve the goals listed above

2.5.3 Lessons Learned

The identification of the models' scope and their priorities needs to be carried out early in the process. This helps getting a focus on the development and delivery of the "Minimal Viable Product" to guarantee the project success.

2.6 Work Package 6 – Communication & Dissemination

Work Package 6 is dedicated to dissemination, communication and exploitation of project results. The goal is first and foremost to boost the impact of the project and its scientific results through effective communication, dissemination and exploitation activities. According to the Grant Agreement the goals of this work package are the following:

- Set-up and apply a dissemination strategy to spread MODALIS² results EU-wide

- Plan and coordinate the participation in conferences, fairs, clustering events and inter-project harmonization, especially synchronization with other H2020 activities
- Identify and implement exploitation mechanisms with the partners and other EU industries to ensure uptake and portability of MODALIS² results beyond the planned applications within the project with consent of the partners owning the respective results
- Summarise the overall MODALIS² outcome in an evaluation report for wide-spread communication validated by all partners
- Plan and coordinate the project's dissemination activities to spread the project results EU-wide, such as participation in conferences, project website, fairs, journal articles etc.
- Contribute to clustering events and inter-project harmonization, especially for synchronization with other activities in the H2020 programme

2.6.1 Achievements

As reported in Deliverable D6.5 "Dissemination/Exploitation Assessment" the project partners represented the MODALIS² project at twelve international and three national conferences and symposia by transferring their gathered results to the scientific community. Furthermore, two scientific papers were accepted in the journals "Physical Chemistry Chemical Physics" as well as "Nanomaterials". Two further papers are planned to be submitted to further scientific journals. Open access was implemented for all peer-reviewed publications.

As for the exploitation the project partners reported a detailed overview of gathered experience/knowledge and planned use of results in D6.5.

Above all, the project has set up a project website, which informs the broader public of the goals and progress (e.g. publications are published on the website): https://MODALIS²-project.eu/en

Further, an interview series was implemented introducing every partner as well as describing the goals and benefits for each project partner.

Last but not least, the project coordinator was continuously in touch with the coordinator of the DEFACTO project (also funded by the same call) in order to create synergies and stay informed about each other's progresses.

2.6.2 Challenges

The biggest challenge for the project was the COVID-19 pandemic and the resulting restrictions and lockdowns which hit the partners unexpectedly hard. The project partners could not enter their companies' premises and hence several activities had to be put on hold. Additionally, initially planned hiring processes were stopped so that some partners were lacking work force. All these obstacles caused tremendous delays and prevented the partners from carrying out the planned activities and thus generating results. Additionally, conferences were cancelled and thus the consortium was lacking opportunities to disseminate and communicate results for more than 12 months. Consequently, as soon as the lockdowns were over and conferences started to take place again, the consortium has set up a dissemination/communication strategy plan including dissemination/communication possibilities and topics relevant for the project. This plan was updated on a regular basis together with the whole consortium during joint meeting.

2.6.3 Lessons Learned

Since a pandemic is hard to predict there is no best practises to prepare for one in terms of project work. After the COVID-19 pandemic, everyone had to learn working flexibly. Hybrid meetings and conferences, home office and flexible working hours have become our normality and almost everyone had the chance to adapt to these new circumstances. The same applies for conferences which are offered in hybrid form allowing everyone to participate remotely. Having a dissemination/communication strategy, which also includes the impact you want to make as well as the stakeholders and users you plan reaching, is crucial right from the start of the project. This also means that the strategy should not be planned last minute but well integrated into the entire grant application Once the project has started, this plan needs a regular update which should be carried out by the whole consortium and should be aimed at maximising the expected impacts. It is therefore important that all partners are and stay informed about what is happening in the project at all stages and in all parts.

2.7 Work Package 7 – Project Management

WP7 is dedicated to project management. It ensures an efficient implementation of the project workplan, monitors risks and is responsible for the communication within the consortium on the one hand, and with the EC and other projects on the other hand.

2.7.1 Achievements

Management of the overall project:

- Implementation of project monitoring
- Organization of regular OMT meetings
- Organization of regular SC meeting
- Organization of General Assembly meetings with the whole consortium
- Continuous monitoring of the risk assessment
    - Many risks were not foreseen at the beginning of the project and mitigation measures were applied regularly.

Due to COVID-19 crisis several issues occured due to communication difficulties within the project.

- No face to face meeting were possible from march 2020 until November 2021
- Initially planned face to face General Assembly meetings were replaced by remote Teams meetings

Successful countermeasures to the above mentioned issues were the following:

- To ensure a better progress management of the project, more regular SC meeting were planned from March 2020 until the end of the project, such meeting were initially dedicated to follow the status of each partner regarding the COVID-19 (company closed, distant work, labs closed...) and then due to technical difficulties to follow the solution for Gen3b cell manufacturing.
- Instead of restricting OMT meeting to Work-Package Leaders, OMT meeting were opened to technical staff of each partners involved in the project in order to improve communication and information sharing.
- Regular joint WP meeting were organised (WP1-3 and WP2-5 and WP4) in order to share the progress between involved partners.

Due to COVID-19 and also technical difficulties 2 amendments were necessary for the project, leading to the involvement of a linked third party from year 2 (to get more resources for the project) and also an 8-months extension of the project (to have enough time finishing the project's tasks).

2.7.2 Challenges

Managing a project with multiple partners is challenging especially when no face-2-face meetings are possible. Even though web-meetings are organised, they are not as efficient for information exchange between partners as F2F meetings.

Changes in technical staff within the consortium partners required more time in order to correctly incorporate the newcomers into the objectives and methodologies planned in the project.

New and unforeseen risks occured or had to be identified (ahead) and feasable countermeasures needed to be discussed and applied.

2.7.3 Lessons Learned

Web meetings are not as efficient as face to face meetings for project management.

Special care is necessary to ensure an efficient follow up of tasks and deliveries especially once people involved in the proposal and/or in the first months of the project leave and are replaced by new staff.

Coordinating a scientific H2020 project requires both management and scientific skills. When difficulties arrise in a WP, project coordinator is needed to decide and make technical choices regarding the sollution to adopt in the same time managment skills are also needed in order to follow closely the projects progress and ensure the righ pushes when needed.

3 Report per Partner

3.1 IFP Energies nouvelles (IFPEN)

3.1.1 Achievements per Partner

- MODALIS² was the first European battery project which was coordinated by IFPEN. This is a first achievement and a major success for IFPEN, enabling us to get easier access to other project consortia.
- Multi-scale and multi-physics modelling, with the addition of the mechanical dimension, required the involvement of different IFPEN departments with varied skills. This created new internal synergies between these departments, each contributing its own skills and ideas to the project.
- From a technical point of view, MODALIS² was the first IFPEN battery project to combine mechanics and electrochemistry, both from a modelling and experimental point of view.
- Finally, MODALIS² was the first project in which future Gen3b and Gen4b technologies were studied and modelled.

3.1.2 Challenges each Partner faced

- MODALIS² was our team‘s first experience of a project coordination, and the project started just a few weeks before the COVID-19 pandemic. It was a huge challenge, as we had to get the project off the ground and launch the first actions in a context of lockdown.
- One of the biggest challenges was finding Gen3b and Gen4b technologies. Indeed, the project was about modelling, not developing battery technologies. Modelling, however, requires access to technologies to study and understand operation and measure calibration parameters. The technologies targeted by the project were at lower TRL levels than expected, which complicated the work considerably.
- From a technical point of view, new experimental methodologies had to be put in place to assess the mechanical aspects of these battery technologies.
- Finally, we had to bring together the various modelling teams (both within IFPEN and between the different partners), who usually do not work on the same scales or physical dimensions.

3.1.3 How will the MODALIS² results be used in your company

- MODALIS² was a project in which new modelling approaches were implemented specifically for future Gen3b and 4b battery technologies. This work has therefore paved the way for generation 3b or 4b battery development projects that require modelling support.
- The results of MODALIS² have already been reused and improved in two projects: The European project HELENA for the development of all-solid-state batteries (Gen4b) in which

IFPEN is the leader of the modelling work package as support for developments, and the French PSPC Régions project Auranode in which IFPEN, using modelling, must improve the production process of Gen3b negative material.

- The results will also soon be reused in the European BATCAT project which has just been accepted for funding. This project, in which IFPEN is WP leader, will make the link between manufacturing and system performance.
- Finally, the work of MODALIS² has raised many more fundamental questions about the modelling of these future battery technologies. These questions have led IFPEN to propose several activities at lower TRL such as those planned in the French PEPR BATMAN project, as well as several associated theses.

3.1.4 Lessons Learned for Future Projects

- Battery modelling projects require battery samples to model. For modelling projects on future technologies, batteries do not yet exist or only as inaccessible prototypes for which the properties and performances are not yet fixed or representative.
- For these projects, it is therefore important and necessary to secure the supply of technologies and to identify several possible and reliable suppliers before the beginning of the project.
- It is also necessary to systematically plan and start the activities with an existing commercial technology. This makes it possible to start modelling work in order to quickly create synergies between the modelling partners and to set up approaches and methodologies.
- The COVID-19 experience has shown the importance of face to face meetings. These meetings are essential to create a group dynamic and a joint identity of the project. They mustn't be underestimated and cannot be replaced by videoconference meetings.
- Finally, the organisation of deliverables must be done to create real synergies between the partners. Thus, the deliverables should not be only compilations of compartmentalised activities. The partners, by working together towards the same objective such as the development of a common model or a common methodology, greatly develop their skills through the sharing of information and know-how.

3.2 SAFT

3.2.1 Achievements per partner

SAFT has experienced a strong collaboration with the MODALIS² project partners. It was a chance sharing information and expertise with all of them.

SAFT was in charge of the Gen3 high Si based anode cell prototyping as well as the preparation of Gen4 cells at the laboratory scale using materials from project partners. The technical expertise in electrode formulation, component compatibilities and electrochemical cycling conditions of the company was confirmed at this scale, even for the new prototype Gen4 cells.

Deep characterisation was carried out on the dispatched cells by IFPEN, Siemens, CRF and SAFT in order to feed the modelling part. The data gathered was used to calibrate the MODALIS² simulation toolchain. The model validation according to use cases has been done under strong collaboration between SAFT, Siemens and IFPEN. As the result, the final models released are operational to simulate complex cells, with blend active materials and specific geometry according to SAFT specific needs.

3.2.2 Challenges each partner faced

Excluding safety incident during cell preparation & experimentation (by partners & subcontractor) despite new technologies involve new hazards and constraints was one of the challenges for SAFT as a cell manufacturer.

At electrochemical level, and more specifically for Gen4, the challenge was to find the optimal formulation conditions with these specific materials that present an important moisture sensitivity. There is always a fine-tuning between the mass ratio, the granulometry and the chemical compatibility of the components. After this optimization part, there are still remaining challenges on the cell assembly conditions, especially in the determination of the pressure to apply.

Regarding the model specification and validation, the selection of the required inputs has resulted in a full reflection to consider all the cell complexity, especially for new technology as solid-state batteries. The model validation part was challenging from the technical point with many inputs required to reach a solid approach on both formation and cycling processes on the silicon/graphite cells. In addtion, the complexity has also been multiplied due to tight planning as model validation was the last task performed in the project.

3.2.3 How will the MODALIS² results be used in your company

The simulation toolchain integrates all the aspects of the batteries from microscopic scale to complete system and provide a better understanding of the new technologies such as Gen3 high Si based anode. A reliable and efficient modelling tool will allow raw material, cell manufacturer and final user to specify and verify the cell performances and cell components by simulation. It saves time and lead time, reduces engineering effort, cost and time related to prototyping and testing. Efficient simulation deployment will be a key differentiator for European battery industry vs. Asian competitors who frequently adopt experimental iterations approach.

3.2.4 Lessons learned for future projects

The delivery and regular reminders of instructions on cell safety limits and cell handling conditions is mandatory to help the partners to work safely, especially with prototype cells.
The anticipation of test set-up for new technology is important to avoid losing resources and time. Indeed, at the time of the first Gen4 batch delivery, due to lack of test set-up for Sulfides in some partners facilities, tests were performed several weeks after the cell reception. This led to the cells' degradation (self-discharge) in the meantime and consequently to a lower performance than expected. However, the second batch cells have been tested immediately after reception and have demonstrated compliancy with expectation.

3.3 SIEMENS INDUSTRY SOFTWARE SAS (SISW)

3.3.1 Achievements per partner

- SISW has increased its understanding of Gen3B and Gen4 battery behaviour thanks to the experimental and modelling activities done in the project.
- Gen3B models have been successfully integrated in Simcenter Amesim and Simcenter Star-CCM+ products.

3.3.2 Challenges each partner faced

- The COVID-19 world-wide pandemic situation also brought in some challenges to recruit the appropriate personnel to address the work in workpackage 5.
  - This caused some delays as to engage the hiring process
  - This was a constraint which wasn't under our control
- Siemens required an agreement amendment to allow for the integration of additional resources into the project coming from Siemens German subsidiary
  - The process took some time, mainly in the hiring process
  - This was completed successfully as the additional resources from Germany could join the project and contribute significantly in D5.2 and D5.3
- Delivery of the derived models from research effort (experimental or modelling) has high impact on the implementation completion. Any delay to the model delivery is a direct consequence on delay for model implementation

3.3.3 How will the MODALIS² results be used in your company

- SISW improved its knowledge on the behaviour of Gen3b and Gen4 batteries, and on the modelling of the main phenomena
- The Gen3b model has been implemented by IFPEN in Simcenter Amesim as a specific new component in the Electric Storage library. It will be industrialised in a future version of Amesim, making it available for our customers in the course of 2024.

The Gen3b model implementation has been completed and integrated into the official Simcenter STAR-CCM+ release codes. This means they will be available for downloads to our customers' base in the course of 2024.

3.3.4 Lessons learned for future projects

- Anticipate the participation of resources with key competencies during the project proposal creation.

- Identify the models' scope and their priorities for implementation early in the process. This helps setting a focus on the development and delivery of the "Minimal Viable Product" first in order to guarantee the project's success.

3.4 SIEMENS AKTIENGESELLSCHAFT (SAGCT)

3.4.1 Achievements per partner

Cyclic ageing for Gen3b cells was investigated in detail at SAGCT. To this end, electrochemical methods (including EIS) were used. Additionally, dilatometry was established to examine the mechanical expansion of the cell during cycling. Different test conditions (temperatures, depth of discharge, state of charge (SOC), rates) were employed to investigate the influence of these parameters on the cyclic ageing. It was possible to examine the data in detail and show that the mechanical expansion of silicon in certain SOC ranges has a pronounced effect on the ageing of the cell. Gen4 full and symmetric cells were also investigated by different electrochemical tests, demonstrating relatively large differences between individual samples of the first Gen4 batch.

3.4.2 Challenges each partner faced

During testing, small differences between Gen3b samples of different production batches became apparent. Therefore, samples had to be exchanged between different partners and the test plan had to be adjusted accordingly. Furthermore, introducing the new method of dilatometry posed challenges for the test setup, which could be solved eventually.

3.4.3 How will the MODALIS² results be used in your company

The measurement data was used for the parametrization and validation of the models implemented by SISW and other project partners. These models will be a useful tool to investigate the performance of next generation cells in the future. Furthermore, the developed test setup combining electrochemical and dilatometry measurements can be applied to battery cell investigations in the future.

3.4.4 Lessons learned for future projects

Batch-to-batch differences and differences between individual samples can influence the obtained measurement data. This particularly affects the ability to extract parameters for modelling purposes which rely on an in-depth analysis of the data. Therefore, the test plans and sample production should be aligned well to avoid unwanted influences.

3.5 UMICORE

3.5.1 Achievements per partner

In this project Umicore was able to translate the cell requirements of MODALIS² partners into material requirements and to develop and sample NMC materials. We were also able to send material to SAFT USA to produce the required cells.

Strong collaboration was achieved especially within WP1 between Umicore as active material provider, SOLVAY as electrolyte provider and SAFT as cell manufacturer. As explained in deliverable D1.4 it allowed MODALIS² partners to develop efficient cells as well as a close to reality virtual model. This model was based on material characteristics information given by Umicore.

Within WP4, there are limited achievements except some knowledge sharing from other partners. We were not able to run the simulator for our use case due to the licensing issues.

3.5.2 Challenges each partner faced

Umicore faced some challenges on the anode side and we were not able to provide SiC active material. Therefore, we had to purchase SiC from a third vendor. After contacts with various SiC suppliers, we were able to identify suitable SiC to be used by SAFT in the project.

Regarding WP4, it took a lot of time to get the licenses, certifications and source code of the software. By the end of the project, we only managed to run Amesim with correct licenses but there was no time to run and validate the model for our use case. The trainings were received well before the software licenses were available and thus not very efficient.

3.5.3 How will the MODALIS² results be used in your company

Thanks to MODALIS², Umicore was able to have access to a cell model. The use of modelling tools from other use cases in WP4 have shown robust results to simulate the cells formation, nominal and ageing conditions in both calendar and cycling models, which were validated for C-rates, HPPC and road tests with the experimental data. For Umicore, the simulation of HPPC and cycle ageing is of great use to study the effect of particle size, electrode thickness, porosity and tortuosity on DCR, DCR growth and cell ageing. This will enable us to develop better materials with lower resistances and higher cyclability.

3.5.4 Lessons learned for future projects

For future European projects, Umicore will only commit to propose material that we are certain we can provide avoiding jeopardising the project. Also, when dealing with cell models, Umicore will prepare more by itself in advance to have Umicore colleagues from various departments more involved from the start. For similar future projects, additional stress should be given on methods of software license sharing and suitable training time for model application.

3.6 RHODIA OPERATIONS (SOLVAY)

3.6.1 Achievements per partner

- MODALIS² was an opportunity for SOLVAY to be linked to industrial players of European Battery Alliance, and to share common methodologies.

- It is the first time a thermo-mechanical with chemical induced swelling was linked to electrochemical model, that requires to link different departments within SOLVAY (characterization, modelling …) what is slightly different from the chemio-thermo-mechanical models we developed up to now. A specific computational workflow has been established within SOLVAY (especially for liquid electrolyte materials, with surfaces and interfaces chemistry).
- From a more technical point of view, this project helped us to benchmark our internal model to others develop by partners, to improve it and to access from the simulations done by other partners (different scales) to accurate parameters.

3.6.2 Challenges each partner faced

- The first challenge was related to the project staff due to the COVID-19 pandemic, its lockdowns and partial unemployment (2020-2021). A part of the activity planned by SOLVAY could not be achieved. Secondly, due to the specific skills (modelling) needed within the project, and personal evolutions (one of the contributor has resigned, another one has been transfered to another service), we could not keep the initial targeted rhythm, on both technical and networking aspects and efficiency of the collaborative work.
- Technically speaking, some difficulties appeared during the project on our capacity to produce the required amount of additives for Gen4b. Although at laboratory level, what was known, the technologies targeted were not at the anticipated yield.
- The technical model is so non-linear that it probably needs to be studied from applied mathematics point of view (stability, convergence, unicity of the solution) in order to ensure the pertinence of the predictions.

3.6.3 How will the MODALIS² results be used in your company

- The new modelling approaches developed in MODALIS² especially at microscale level have complemented the existing know-how of SOLVAY (especially DFT on material level). This new skill will help us first to speak the same language (e.g. more data for product datasheets) as our customers and second to virtually test some formulations to better anticipate how the cell will behave at our customer lab and to align our developments accordingly.
- The experimental methodologies developed will be reused in other projects to better characterise the products.

3.6.4 Lessons learned for future projects

- MODALIS² was very ambitious and the 2 targeted technologies have actually a lower TRL than expected even at the end of the project leading to the difficulty to be provided with samples. The real capacity to produce a specimen is a non-modelling task what could be a specific project, upstream to the modelling project itself.
- Make R&D on mathematic model and physics laws requires using high TRL material to access to realistic values of the model parameters.

3.7 GEMMATE TECHNOLOGIES SRL (GEM)

3.7.1 Achievements per partner

The comprehensive multiscale model developed with MODALIS² project is a showcase of the benefits found in combining a multitude of approaches in a single investigation. The focus on multiscale link for a variety of modelling scales was able to deliver interesting results for each scale and the whole project by combining the strengths of each individual computational technique. Coupling the use of ab-initio DFT codes and FEM-based modelling GEM aims to bridge the gap between the atomistic-scale chemical information and the physical models which are the standard for battery simulation in industrial setting. Specifically, GEM is now capable to exploit DFT modelling results within mechanical, diffusion and thermal models of Li-ion batteries within which those materials are used.

3.7.2 Challenges each partner faced

The complexity of the materials used in the project is hard to convey at a molecular level; as this complexity is reflected on the quantum-mechanical calculations performed by GEM, very long computational times are required to capture the chemical properties which are driving the performances of those materials. Similarly, at the mesoscale, a wide range of parameters within the calculations, such as phenomena, geometries, and boundary conditions, need to be tailored to make the model suitable for a FEM-based multi-physics simulation, so that appropriate levels of stability and computing power demand are achieved.

3.7.3 How will the MODALIS² results be used in your company

The MODALIS² project brought a wide range of new competencies in the field of predictive tools for battery performances and ageing of battery materials. This know-how will promote the participation in new collaborative research projects and enrich the competencies exploitable in direct consultancy activities. Moreover, the exploitation roadmap foresees the co-design of prototypes for existing and new clients, taking advantage of the enhanced expertise developed during the project.

3.7.4 Lessons learned for future projects

The results achieved in the project proved the potential of designing models for chemical systems by integrating ab initio studies and mechanical investigations of different scales. Each model system is capable to provide insight into the degradation processes of the silicon-based anode and produced data for larger-scale models. These parameters are difficult to obtain experimentally, due to the nature of the materials and their interactions during battery operation, so their accurate theoretical evaluation is of fundamental importance. This is a very important but understudied niche, which allows for finer-detail characterization of the materials but requires skills and knowledge from a wide range of very different disciplines, which unfortunately are rarely brought together.

3.8 CENTRO RICERCHE FIAT SCPA (CRF)

3.8.1 Achievements per partner

CRF was involved in different WPs and reached different achievements during the MODALIS² project:

- Cycling of Gen3b cells was investigated in particular by applying WLTC profiles also with fast charge profiles to investigate different behaviors during cycling. Calendar ageing was also performed at different temperatures to monitor the capacity loss during time.
- Gen4 half and full cells were characterised through HPPC and C-Rate test to evaluate the performances. EIS was also performed.
- Lot of effort was put in the development and validation of the simulation toolchain in WP4

3.8.2 Challenges each partner faced

Gen3b cells tested with WLTC profiles lasted few cycles and rapidly the capacity faded. The first batch produced for Gen4 was delayed due to cell assembly issues and the overall performances were lower than expected and planned. The second batch behaved better with more reproducible results and characteristic near the one defined during the cell production.

Better communication between partners can be useful to avoid time losses and misunderstandings that can affect the project results.

3.8.3 How will the MODALIS² results be used in your company

Thanks to MODALIS² project CRF gained several skills on different aspects:

- A better understanding of the Gen3b and especially Gen4 cells, regarding performances and cyclability
- The simulation toolchain developed in the project showed the importance of numerical simulation for the lithium-ion batteries field, a powerful tool that can help industrial realities.

3.8.4 Lessons learned for future projects

The cell behavior can be highly influenced by the protocols applied and in order to avoid uncertainties common protocols must be defined at the beginning of the project, like what was done in MODALIS². The collaboration between simulation tools and experiments can push forward the research on the battery field, allowing industries and companies to evolve their capabilities.

3.9 UNITO

3.9.1 Achievements per partner

UNITO was mainly involved in WP2 and WP3. Regarding WP2, UNITO successfully developed a suitable computational protocol for the ab initio estimate of diffusion coefficients in cathode and electrolyte materials, which involves the use of multiple computational tools combined. Moreover, it developed successful models for solid electrolyte materials, surfaces and interfaces, and modelled several chemical and physical processes happening on the atomic scale at the interfaces. Regarding WP3, UNITO performed NMR and Raman measurements on Argyrodite materials, and successfully compared theoretical models with experimental results. All of this led so far to two published papers, one submitted and two under preparation.

3.9.2 Challenges each partner faced

The main challenge in the first year of the project was related to the COVID-19 emergency. Networking, both internal and external, and recruitment were severely impaired in this timeframe. In the following, the main challenges were due to the complexity of the systems under study, which resulted in: 1) additional work in setting up and testing the atomic-scale models and 2) computational requirements (processors, memory) higher than initially estimated.

3.9.3 How will the MODALIS² results be used in your company

UNITO has greatly improved upon its know-how related to Gen3b and Gen4 batteries. New computational tools have had to be learned beyond the Crystal program, bringing the UNITO team out of its traditional comfort zone. Internal and external networking has greatly improved, with important synergies between experiments and theory. All this knowledge will be fruitful for future projects as well as for the development of new models and algorithms.

3.9.4 Lessons learned for future projects

The diffusion coefficient, a key quantity to our approach to battery modelling at the atomistic scale, remains something that is hard and challenging to predict, simulate and measure. This calls for new computational tools and/or transport theories. From the project management side, we learned a lot on the functioning of large projects with a strong industrial partnership.

3.10 K&S GmbH PROJEKTMANAGEMENT (K&S)

3.10.1 Achievements per partner

Over the past 20 years, K&S has supported scientists in various disciplines and companies in securing public funding for many collaborative projects. Our multi-disciplinary and highly qualified team has many years of experience notably in projects in Automotive, Energy and ICT. Besides the expertise in administrative project management, communication and dissemination, our team is completed by in-house graphic design experts. Especially due to the COVID-19 pandemic, K&S gained additional knowledge in project management as well as communication/ dissemination of project results under „difficult conditions“. A close monitoring of progress and cooperation with all project partners were very fruitful.

3.10.2 Challenges each partner faced

The biggest challenges in this project were the different circumstances due to the COVID-19 pandemic. Initially, no communication activities were possible due to the worldwide lockdowns. Additionally, the lockdowns caused delays of results which caused delays of several dissemination activties. After the lockdowns were finished a ramp-up phase was necessary and the consortium elaborated a dissemination roadmap which was updated on a regular basis. These delays of the first 18 months could hardly be made up for. However, as soon as the first results werde generated the consortium put a lot of effort to disseminate these results to the broader scientific public.

3.10.3 How will the MODALIS² results be used in your company

At K&S, internal Lessons Learned workshops are carried out after each project end together with the whole project management team. As described in the previous section, K&S as well as the whole project consortium had to work in difficult conditions. The way the project dealt and overcame these obstacles will be communicated and analysed internally at K&S.

3.10.4 Lessons learned for future projects

Proper communication, dissemination and exploitation activities take up a lot of time and effort. The goal of K&S is to take a lot of the workload off the other project partners’ shoulders, leaving them more time to focus on the science and innovation. Therefore, it is crucial to elaborate a fitting and detailed communication/dissemination/exploitation plan already during the proposal phase. The project partners should not see this plan as something separate from their core tasks. Hence, everyone needs to agree on this plan and stay informed about what is happening in the project at all stages. Continuously updating each other on activities and results will promote interdisciplinary publications and other dissemination, communication and exploitation efforts.

4 Conclusion

MODALIS² project was aiming at providing new modelling methodologies and tools for next generation of batteries. To do so, its work plan has been devided into 7 work packages (WP) and 10 partners were gathered to fulfill this goal.

Managed by WP7, WP objectives were achieved to provide each other with material, data, models, information. As planned, WP1 provided materials to be tested in WP3. Fit for purpose testing was implemented in WP3 and performed among partners to provide WP2 with information on tested materials, and WP4 on its behaviour. WP2 models were developed from atomistic until full cell level and those models were then implemented in WP5 into Simcenter StarCCM+ and Simcenter Amesim softwares. All these models were then validated in WP4.

This work led to dissemination activities within WP6 where specific care was taken to ensure a better dissemination after COVID-19 issues in the first years of the project.

Many challenges were faced throughout the project with especially COVID-19 which prevented efficient communication within the consortium. Then aiming at future battery technologies is a major challenge as materials are not working according to what is expected and their integration is more complicated. Then their modelling still raises many new questions as they exhibit new unexpected behaviour as we use them.

Nevertheless, MODALIS² was able gathering an original consortium to develop a new toolchain for next generation batteries. Such new tools are already used in consortium's further projects and can provide useful knowledge to the whole European battery industry.