



# Lab of the Future for battery materials research

EMIRI workshop June 30<sup>th</sup>, 2022

# Lab of the future

## A Cross-Program Disruptive Approach Built on 3 Pillars


Why?

Ensuring leading position by providing battery material and application with a disruptive speed (x5)

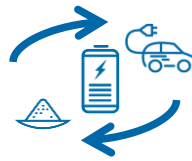
How?

- Internalize critical digitalization know-how
- Create partnership for HT material screening
- Establish in-house multiscale battery and process modelling
- New collaborations for dedicated competence development
- Build modern infrastructure and data systems

What?



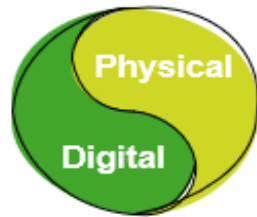
HT material screening using robotization



Multiscale battery digital twin



Process models for all major processes



**Digital HT and autonomous platform** to accelerate first-quality battery material/system development

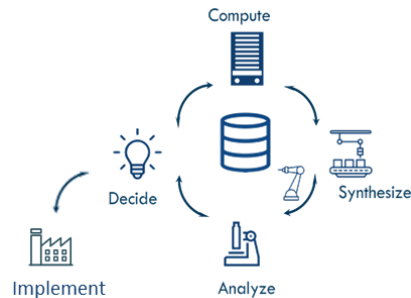
**Multiscale battery digital twin** to understand, quantify and predict battery performance in real-world conditions in order to

- *Extend battery lifetime*
- *Increase efficient use of technologies*
- *Optimize for specific applications/operating conditions*

**Process models** to create fundamental insights, accelerate upscaling and continuously improve mass production

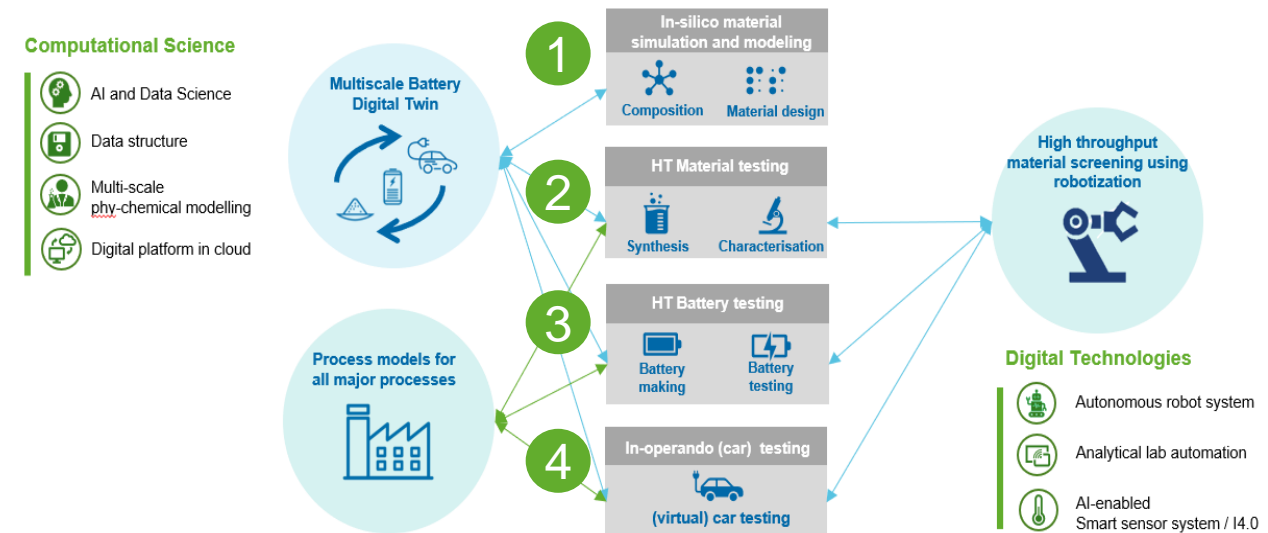
# Disruptive approach making material research faster and cheaper

- Battery material research in four steps:
  1. Chemical composition and material structure design
  2. Material synthesis and characterisation
  3. Battery making and testing
  4. In-car battery testing
- Between those steps are many feedback loops and a lot of parameters to be considered and analysed.



- Conducting all these steps manually cost a lot of time and people.

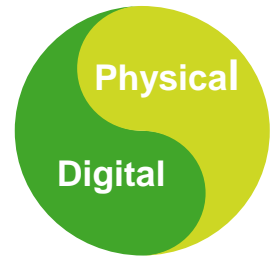
**Computational modelling and robotization can have an impact on all steps of the battery materials research**



Lab of the Future is about leveraging digital twins (modeling) for materials & processes, and robotization (automation & high-throughput) to accelerate the battery materials research at reduced costs

# Our Approach: Lab of the Future

A digital platform for disruptive physical speed

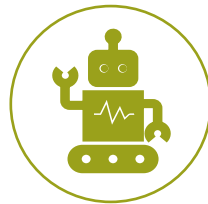


A **multi-scale platform** to increase the **speed** and **scalability** of material research and reveal **complex new insights** in a **closed and autonomous loop**



## Multi-scale battery modeling

Precise understanding (nano- via meso- to micro-scale) for battery performance prediction & application knowhow



## Autonomous robot system

Flexible automation for high throughput synthesis, characterization, and battery testing



## Digital platform

Data storage, autonomous design of experiment, and interaction with lab automation control platform



## AI-enabled sensor

Application for in-situ and in-operando data acquisition during the chemical processes in real time



## Hybrid (AI & Phy-Ch) Model

Explore hidden relationship between complex process parameters and battery performance



## Lab automation control platform

Software-defined automation control by managing mobile robot and automation processes for fully automatized lab

Enable **scalable** battery material research programs

Factors for success: (i) Ramp up critical knowhow, (ii) Twin experimental and digital research teams, (iii) Establish a network of strategic partners

# Lab of the Future

## Reflection

- The program was launched 6 months ago, but Umicore has been already working on modelling related and computational science activities since years.
- Global initiative and external partnerships ongoing.
- **Increase R&D output significantly without increased cost:** Multiproject program involving different and multidisciplinary teams at Umicore on-going
- The common roadmap shows everyone involved how they can contribute.
  - Robotics: Increase lab throughput by automating routine tasks.
  - Battery Modelling: Simulate battery performance based on known material properties.
  - Process Modelling: Breathe life into fundamental process and product understanding. Helps in upscaling effort



materials for a better life

**We are hiring!**

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