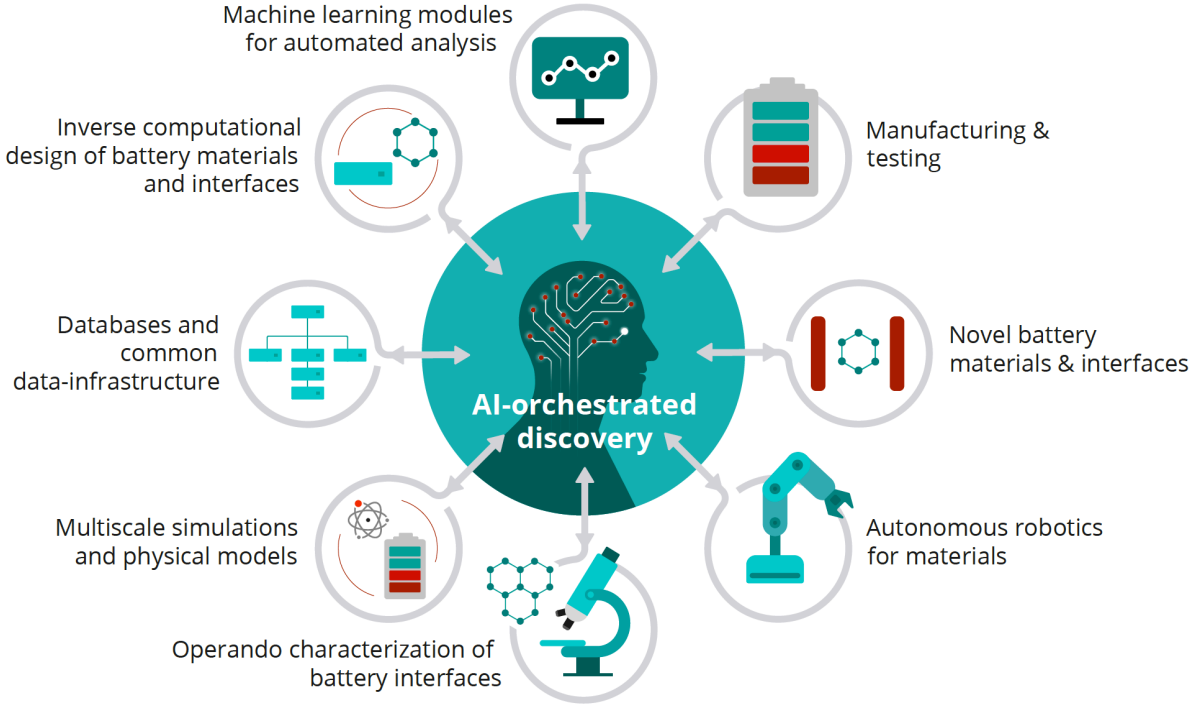
BIG-MAP: Battery Interface Genome Materials Acceleration Platform

1st Stakeholder Webinar



Prof. Tejs Vegge (big-map@dtu.dk, @BIGMAP_EU, www.big-map.eu)

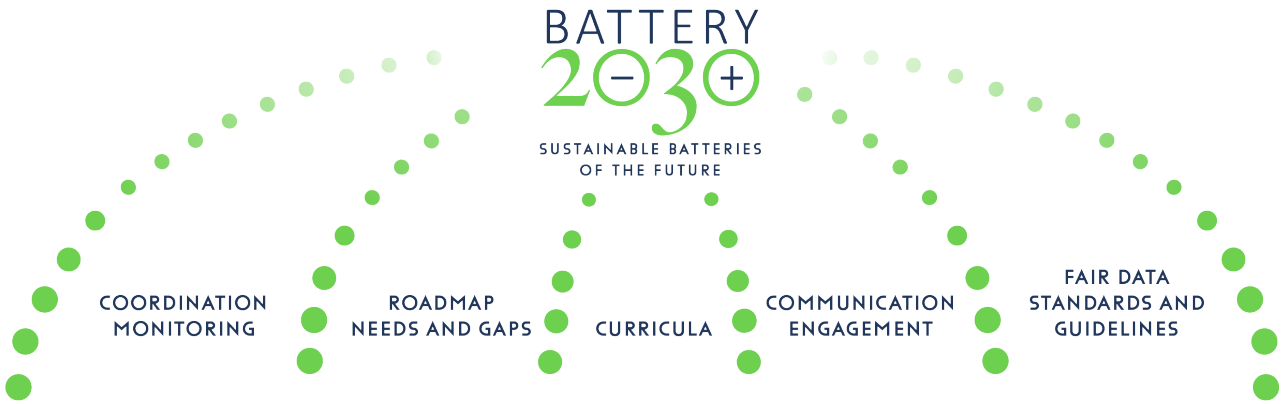
Technical University of Denmark

DTU Energy, Technical University of Denmark

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 957189

BIG-MAP is part of BATTERY 2030+

LARGE-SCALE RESEARCH INITIATIVE



BIG-MAP

BATTERY 2030PLUS CSA
UU, SWEDEN

HIDDEN

INSTABAT

BAT4EVER

sensibat

SPARTACUS

Coordinator:

Kristina Edström, Uppsala University, Sweden

Deputy coordinator:

Simon Perraud, CEA, France

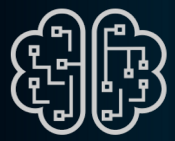
www.battery2030.eu

Twitter: @2030battery

Linkedin: batteryinitiative

BATTERY 2030+

Ultrahigh performances



Smart functionalities

Environmental sustainability

www.battery2030.eu

BATTERY 2030+ - a large-scale research initiative: Inventing the sustainable batteries of the future

Our aims are:

To invent ultra-high performance batteries that are safe, affordable, and sustainable with a long lifetime

To provide new tools and breakthrough technologies to the European battery industry throughout the value chain

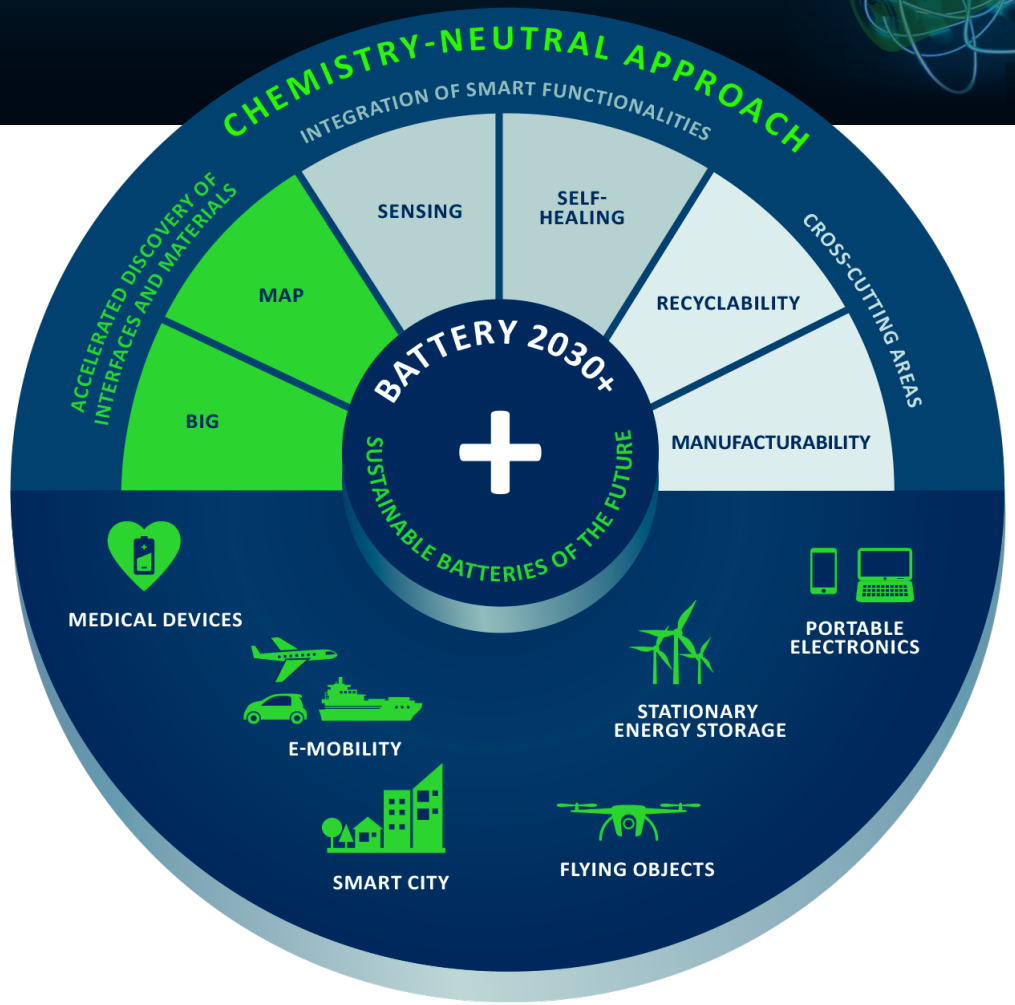
To enable long-term European leadership in both existing markets (i.e., road transport, and stationary storage) and future emerging applications (i.e., robotics, aerospace, medical devices, and Internet of things)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 957213.

BATTERY 2030+ Roadmap
The Research Projects

Versatile and chemistry neutral approach

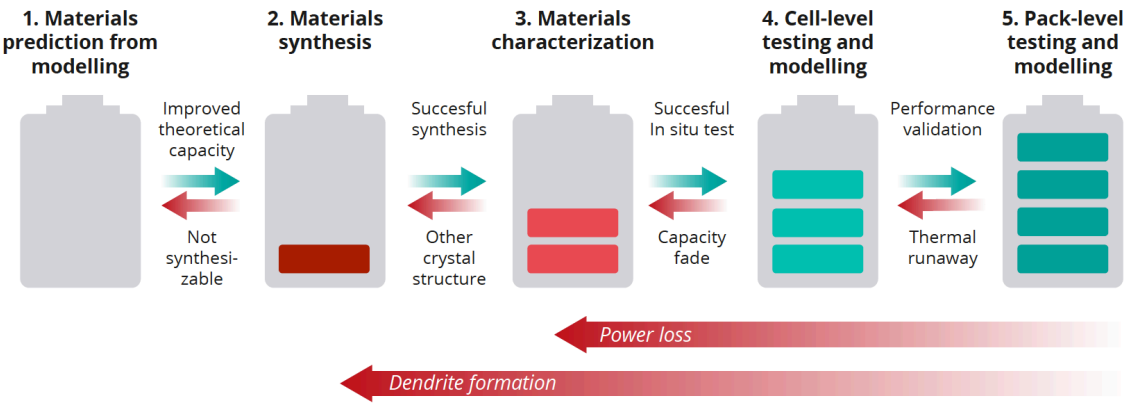
- **Accelerated discovery of battery interfaces and materials** – BIG-MAP (DTU)
- Integration of **smart functionalities** – sensing INSTABAT (CEA), SENSIBAT (IKERLAN) and SPARTACUS (Fraunhofer) and self-healing BAT4EVER (VUB) and HIDDEN (VTT)
- **Cross-cutting areas** – manufacturability and recyclability

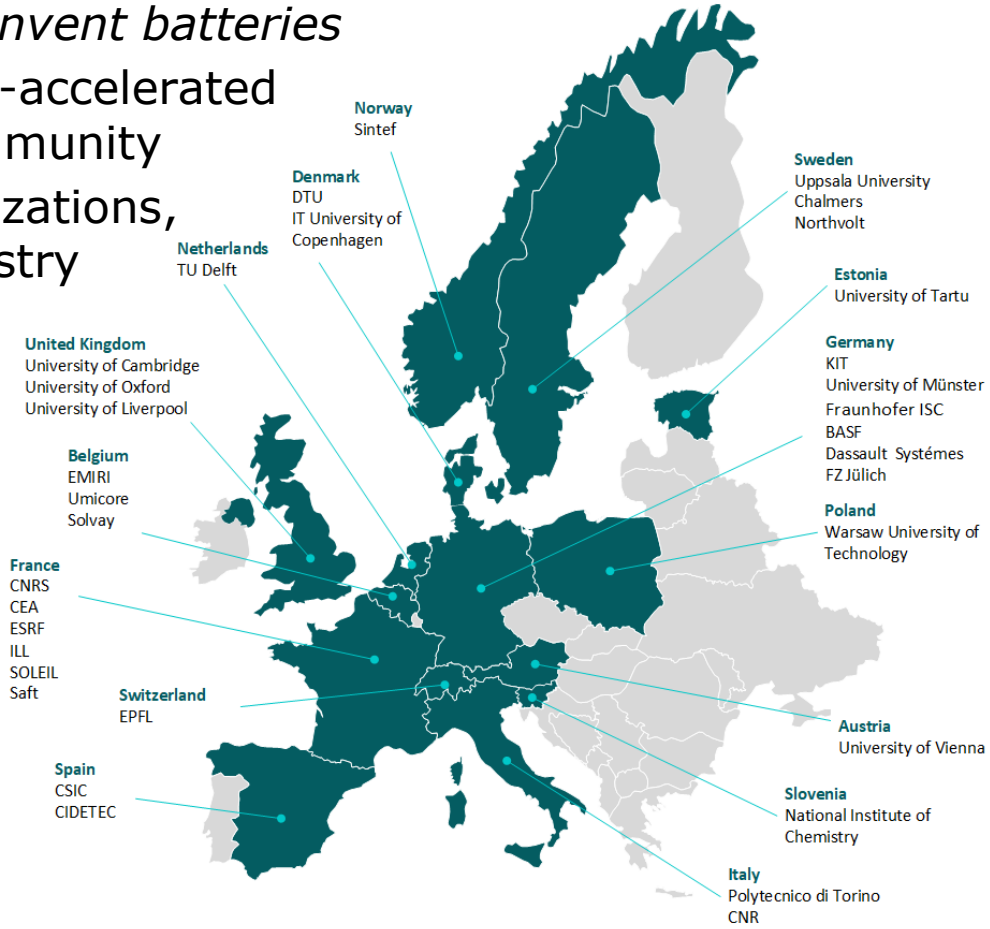


Edström, Dominko, Fichtner, Otuzewski, Perraud, Punckt, Tarascon, Vegge, Winter, BATTERY 2030+ Roadmap (2020)

The BIG-MAP consortium

- 10-year ambition: *Reinventing the way we invent batteries*
- Year 1-3: the first steps in developing an AI-accelerated infrastructure for the European Battery Community
- 34 partners from academia, research organizations, large-scale research infrastructure and industry
- More about the partners: www.big-map.eu





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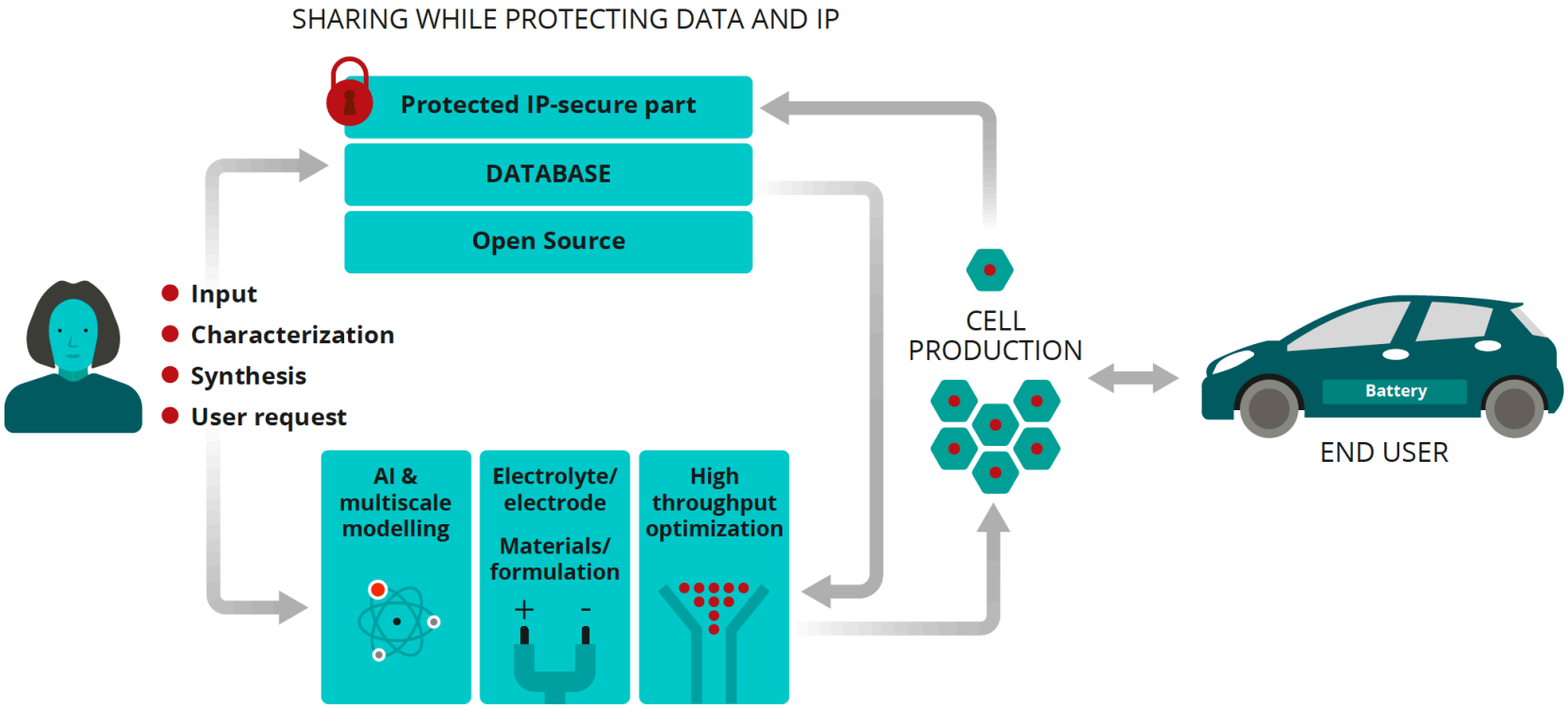
Accelerated Battery Development Processes

- **Vision**: A modular and chemistry neutral platform for accelerated closed-loop discovery using AI-accelerated models & procedures



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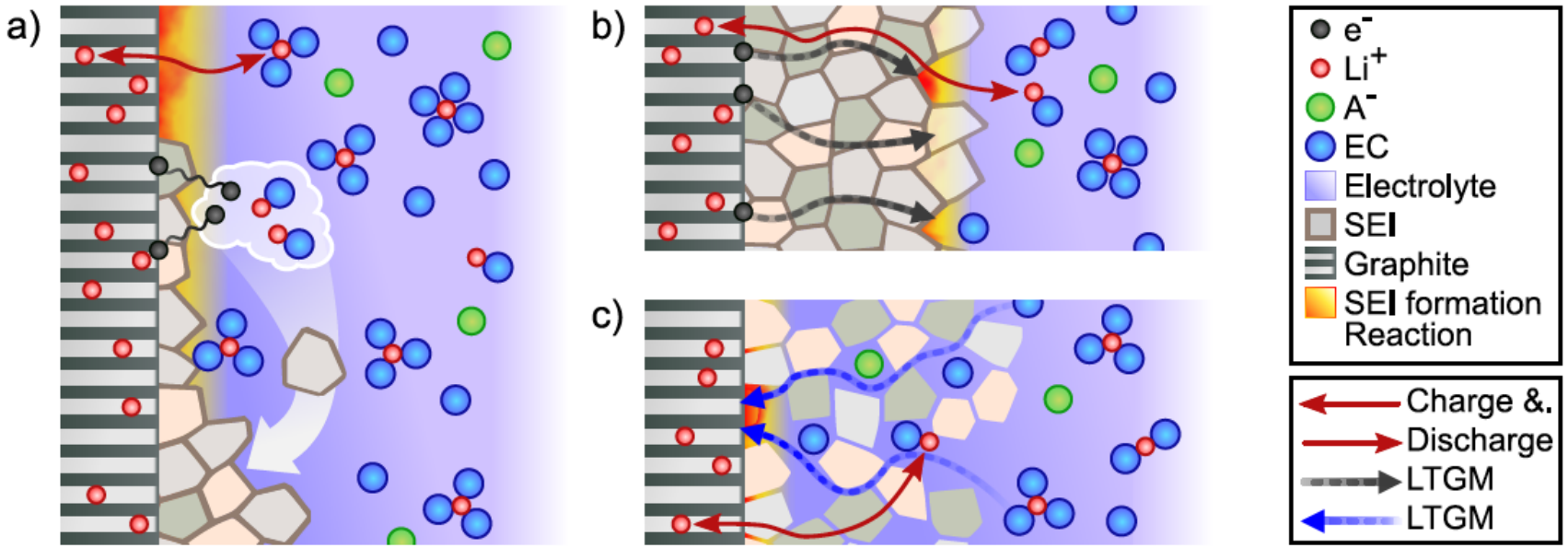
BIG: Understanding & Controlling Interfaces

- Interfaces and interphases play a critical role in all battery technologies
- Physical understanding is essential to develop models for accelerated discovery



Horstmann, Single, Latz, Current Opinion in Electrochemistry 13, 61-69 (2019)

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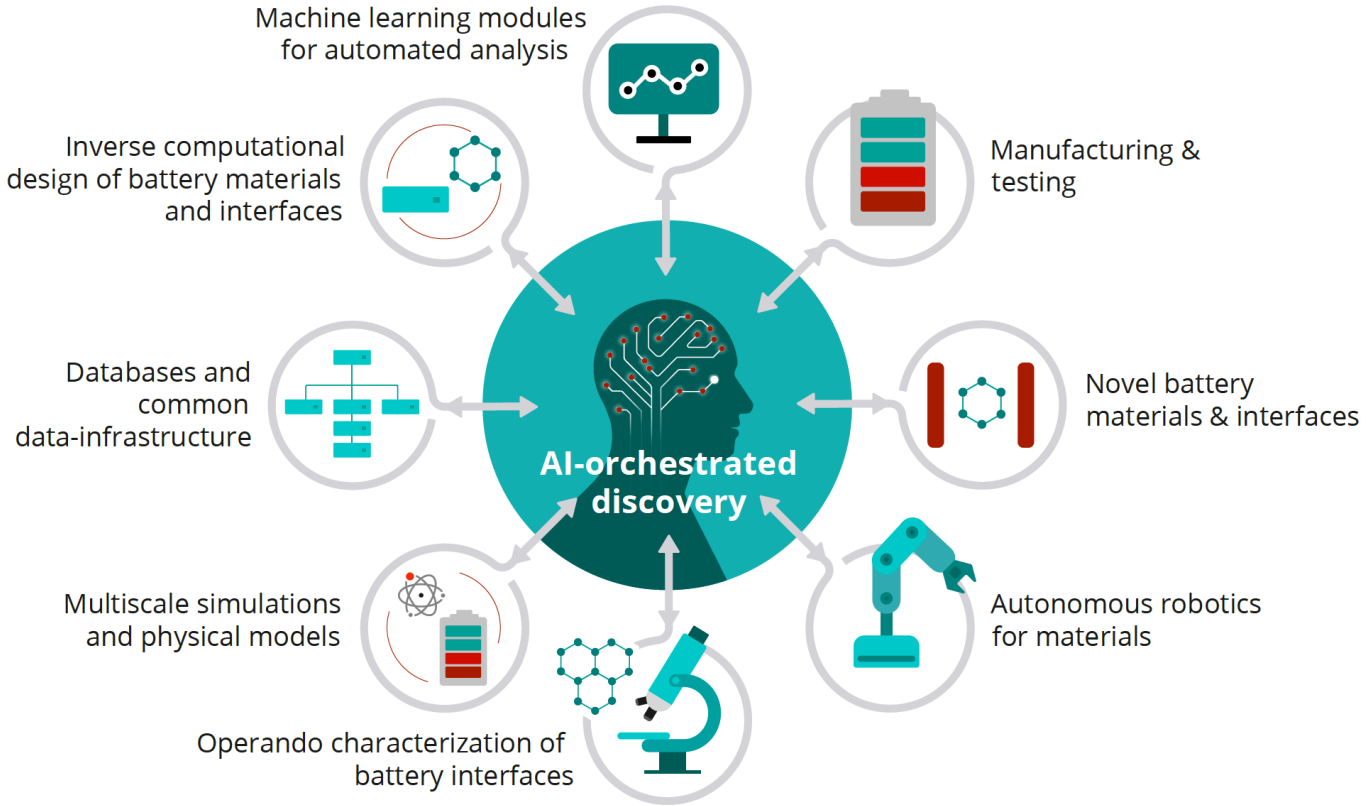
MAP: An AI-orchestrated Discovery Process

- **Mission**: Enabling automated data acquisition, analysis, prediction and utilization



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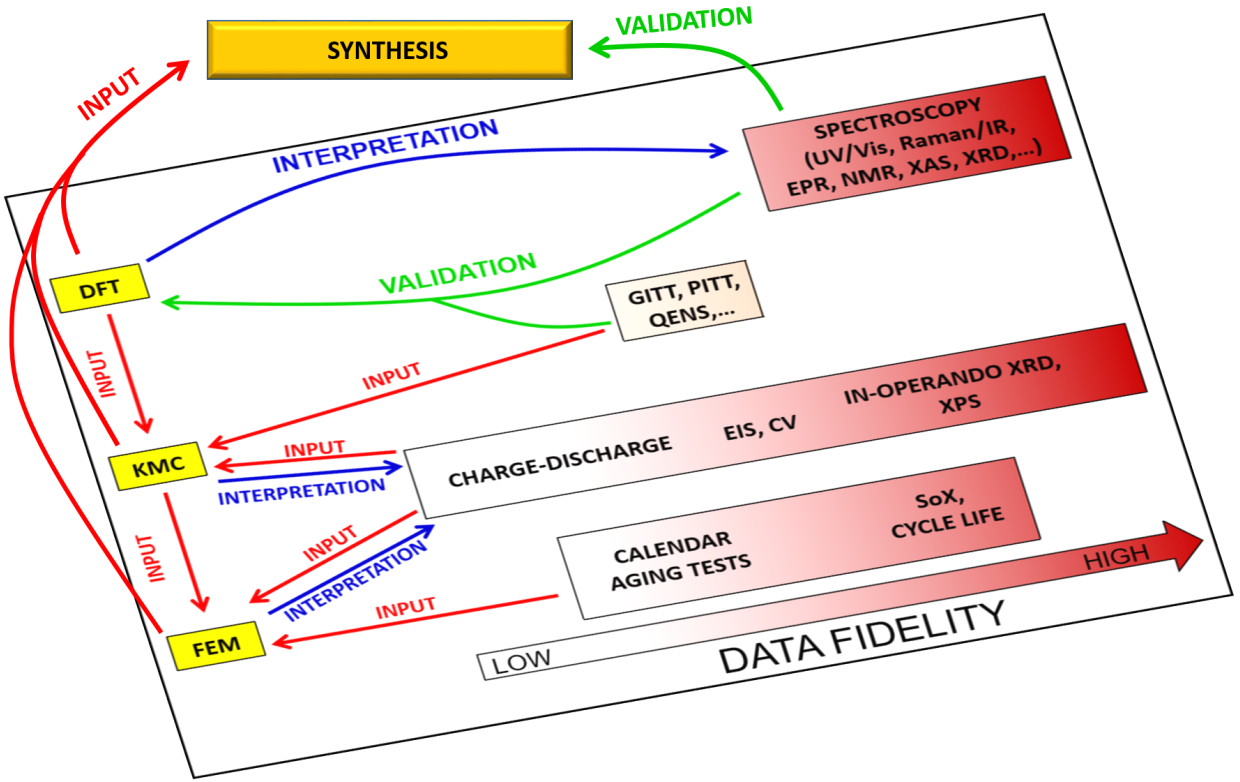
Bridging Scales in Theory & Experiments with AI

- Advanced scale-bridging for prediction of the spatio-temporal evolution of interfaces



Bhowmik, Castelli, Garcia-Lastra, Jørgensen, Winther, Vegge, Energy Storage Materials 21, 446-456 (2019)

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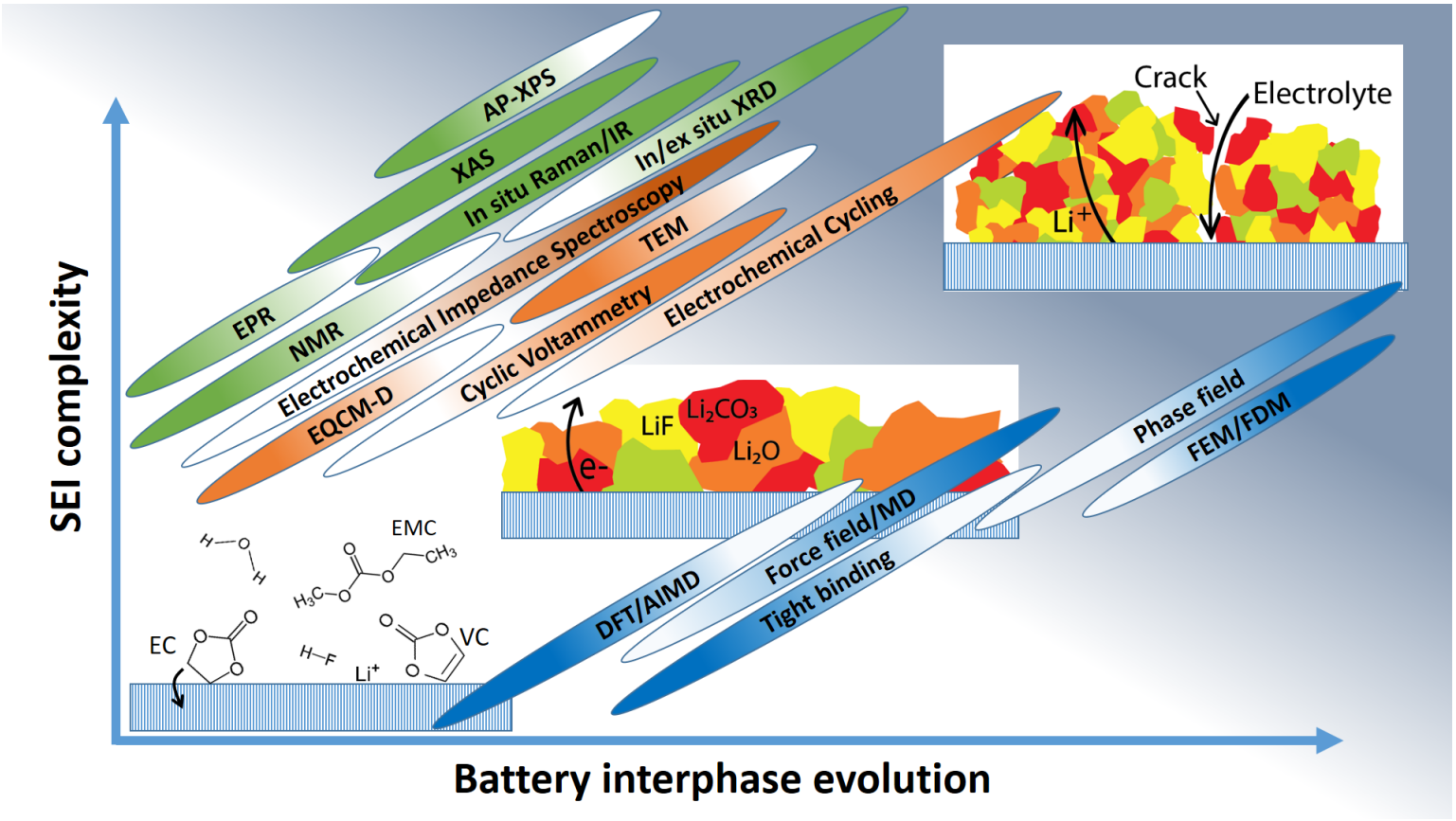
Multi-sourced and Multi-fidelity Data



Bhowmik, Castelli, Garcia-Lastra, Jørgensen, Winther, Vegge, Energy Storage Materials 21, 446-456 (2019)

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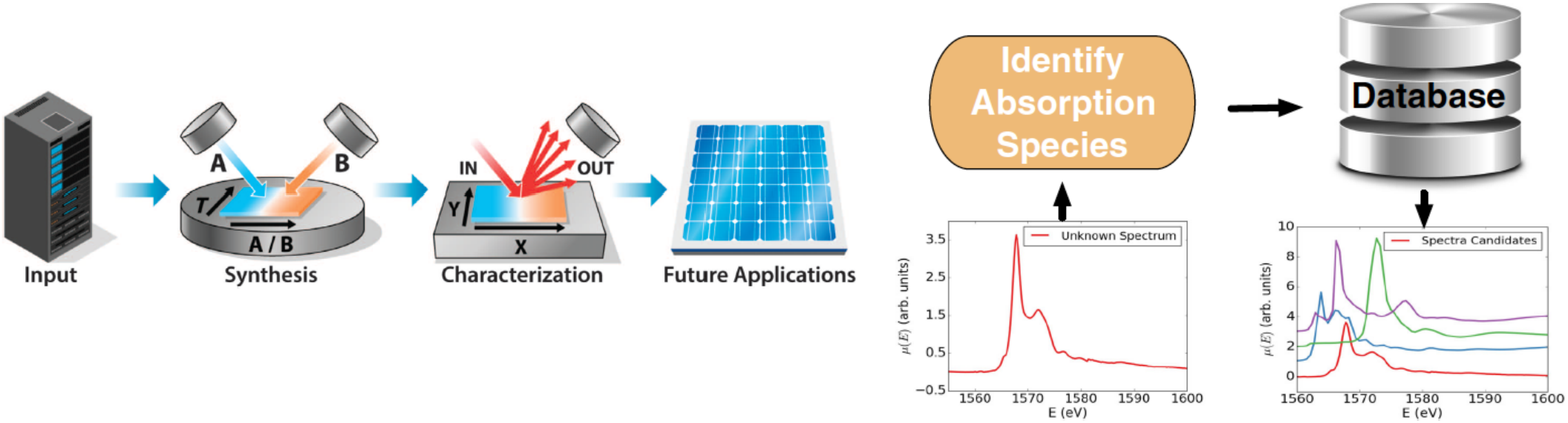
Multimodal Autonomous Characterization

- Integrating high-fidelity (large-scale facilities) and high-throughput (lab-scale) experiments
- Multimodal characterization techniques and ML-modules for autonomous data-analysis



Zakutayev et al, Sci Data. 5:180053. doi: 10.1038/sdata.2018.53 (2018); Zheng et al, npj Computational Materials 4:12; doi:10.1038/s41524-018-0067-x (2018); Suhram et al, ACS Comb. Sci. 19, 37-46 (2017); Stein et al, Chem. Sci. 10, 47 (2019)

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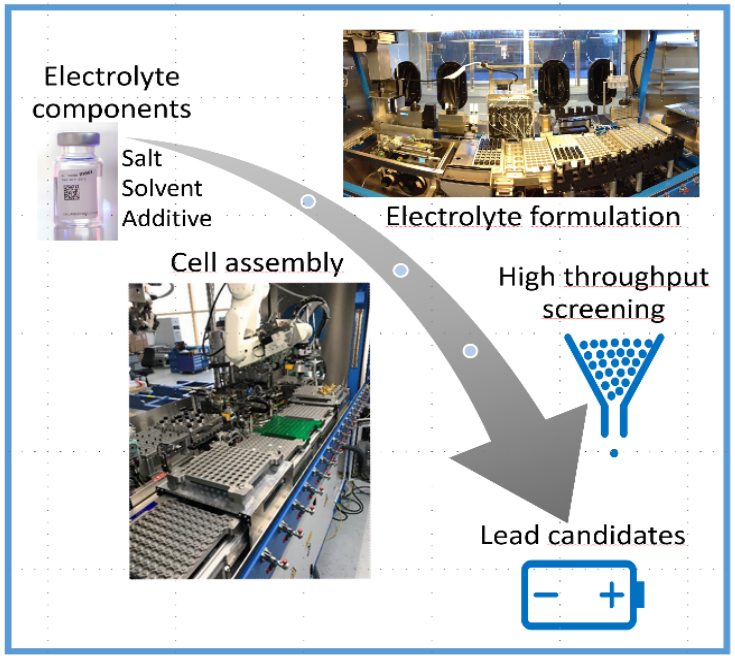
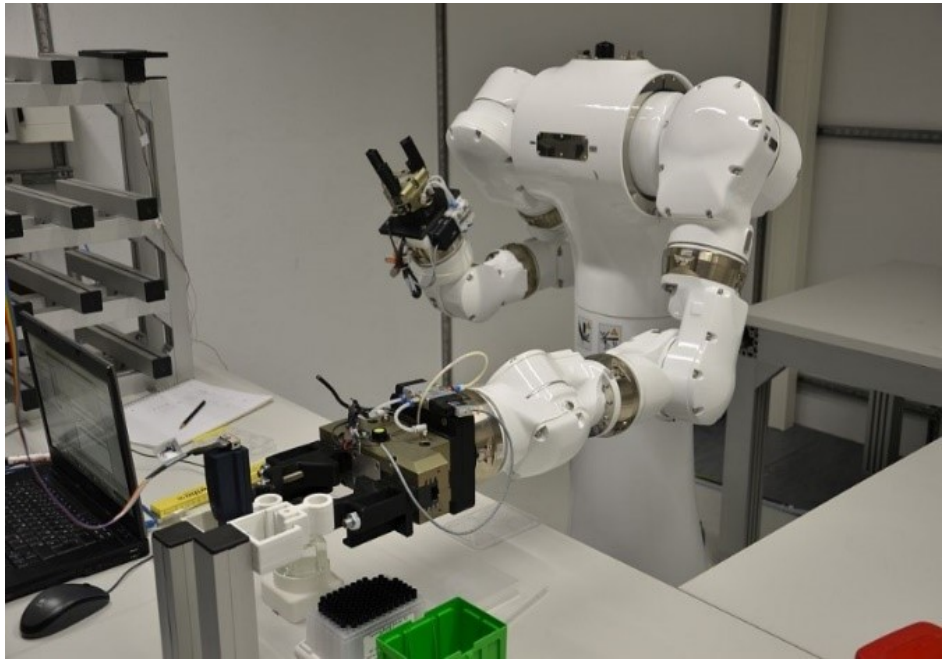
High Throughput Screening (HTS) Systems

- Fully automated HTS systems, e.g., for electrolyte formulation
- Developing autonomous ML-based analysis and orchestration modules





Fully automated HTS system at the WWU/HIMS, for electrolyte formulation, cell assembly, and electrochemical measurements

2-arm robot for wet-chemical synthesis and testing of nanoparticles for medical applications at the Fraunhofer ISC, Würzburg

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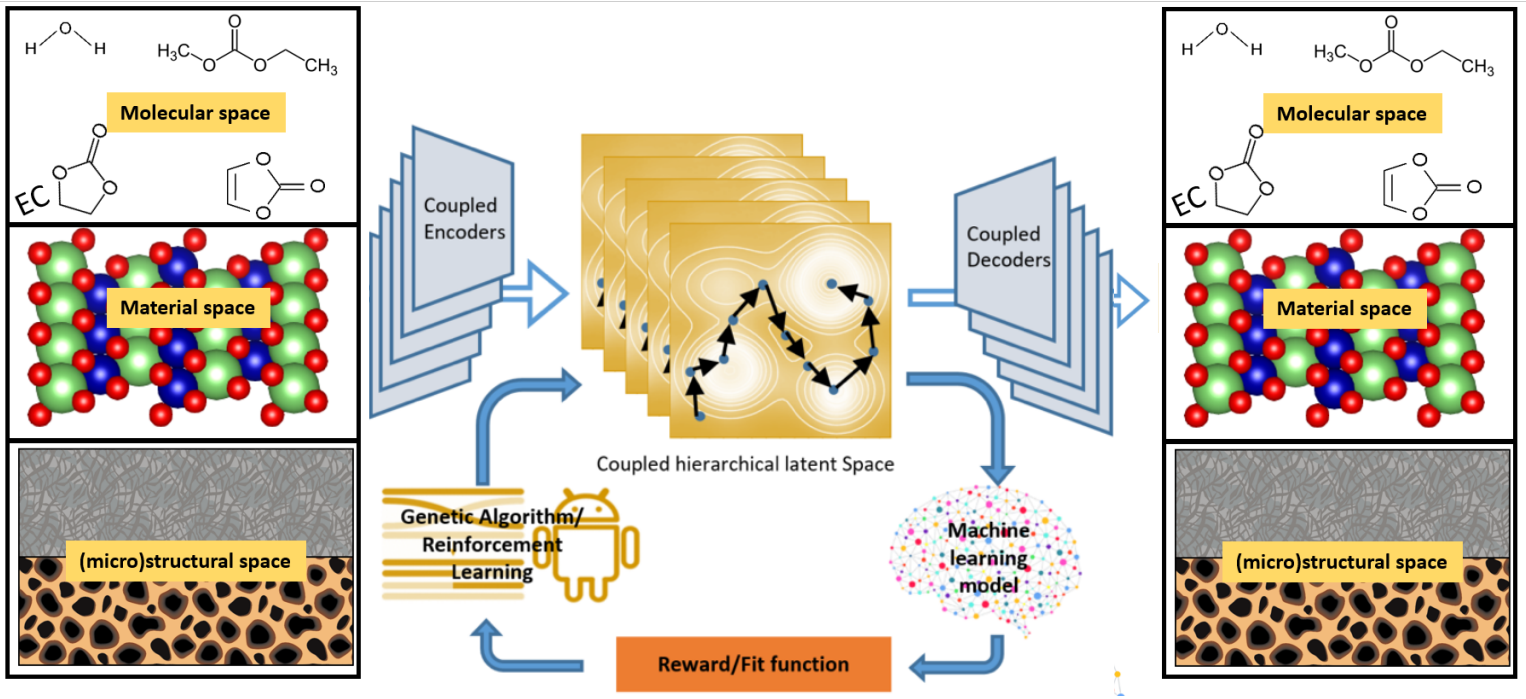
Identifying Dynamic Interface Descriptors

- Inverse design of battery interfaces with spatio-temporal multiscale models
- Generative deep learning to identify dynamic interface descriptors



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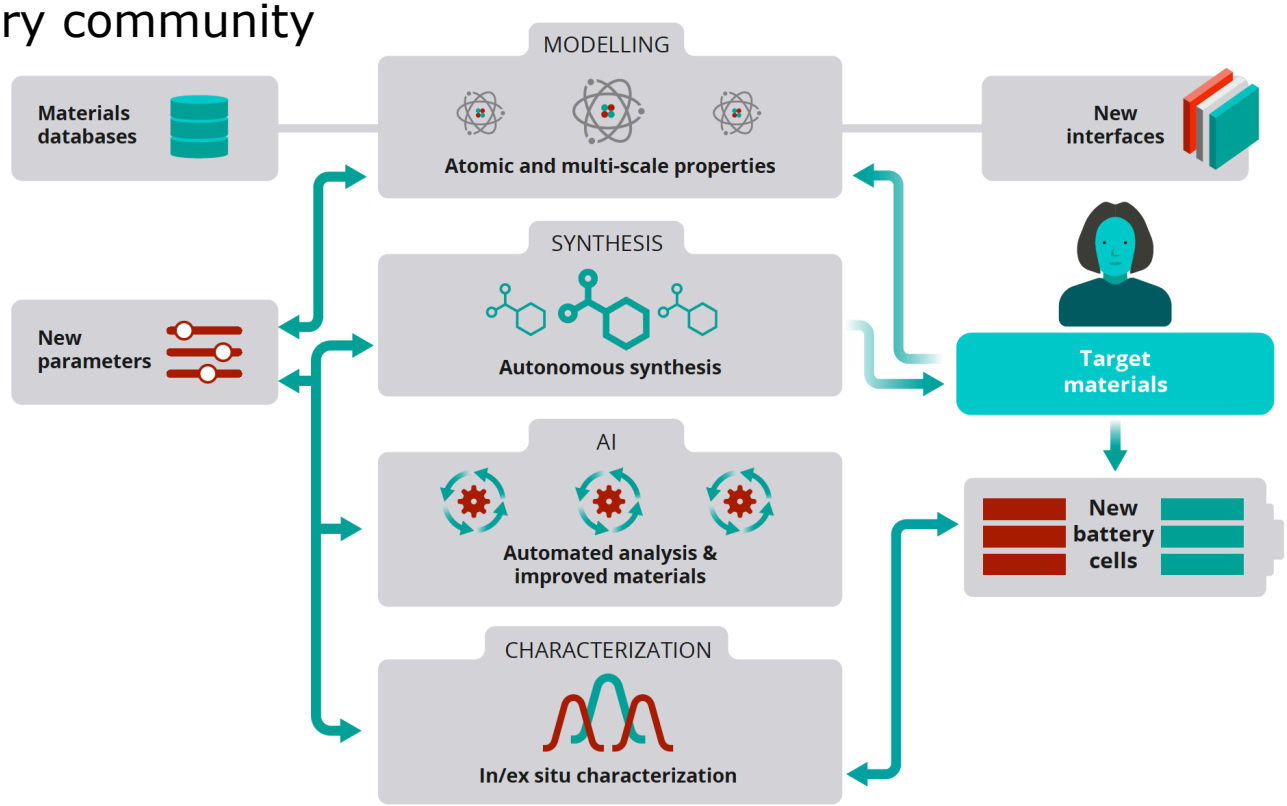
Integrated Autonomous Discovery Workflows

- Developing and sharing workflows and APIs for bridging domains and data in the European battery community



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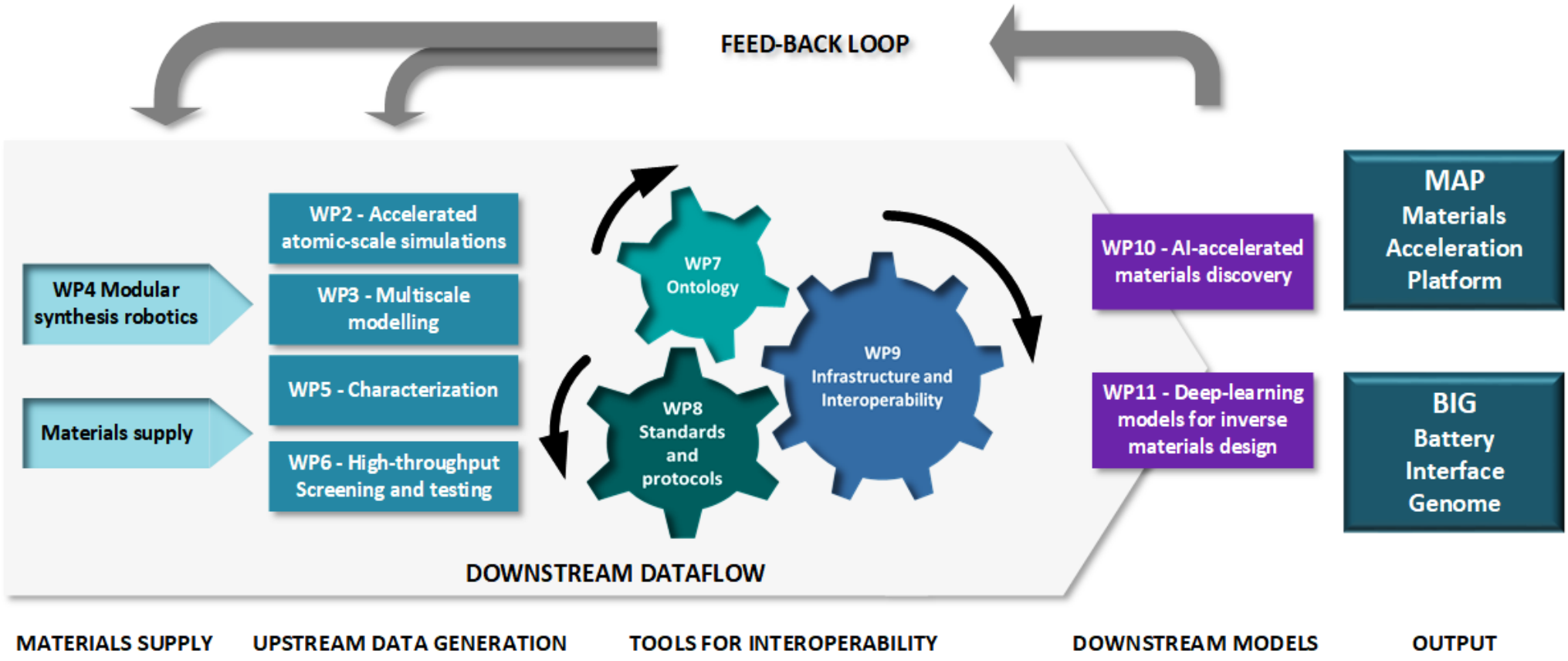
BIG-MAP Data Management Plan (DMP)



Ivano Castelli and Hanne Lauritzen (DTU)

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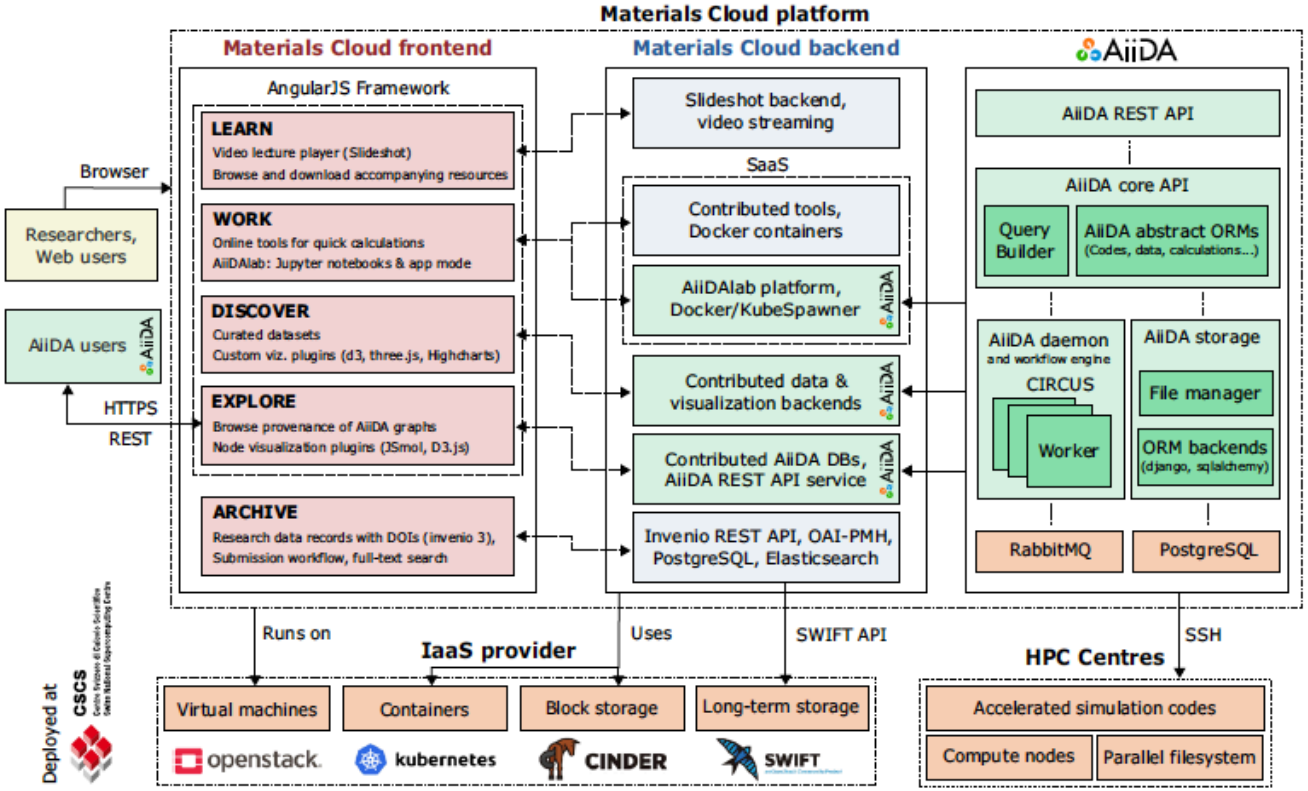
Shared Data Infrastructure & Interoperability

- A shared ontology and data-infrastructure with full data lineage and provenance, across simulation codes, scales, experiments and domains



Talirz et al., Scientific Data 10.1038/s41597-020-00637-5 (2020); Huber et al., Scientific Data 10.1038/s41597-020-00638-4 (2020)

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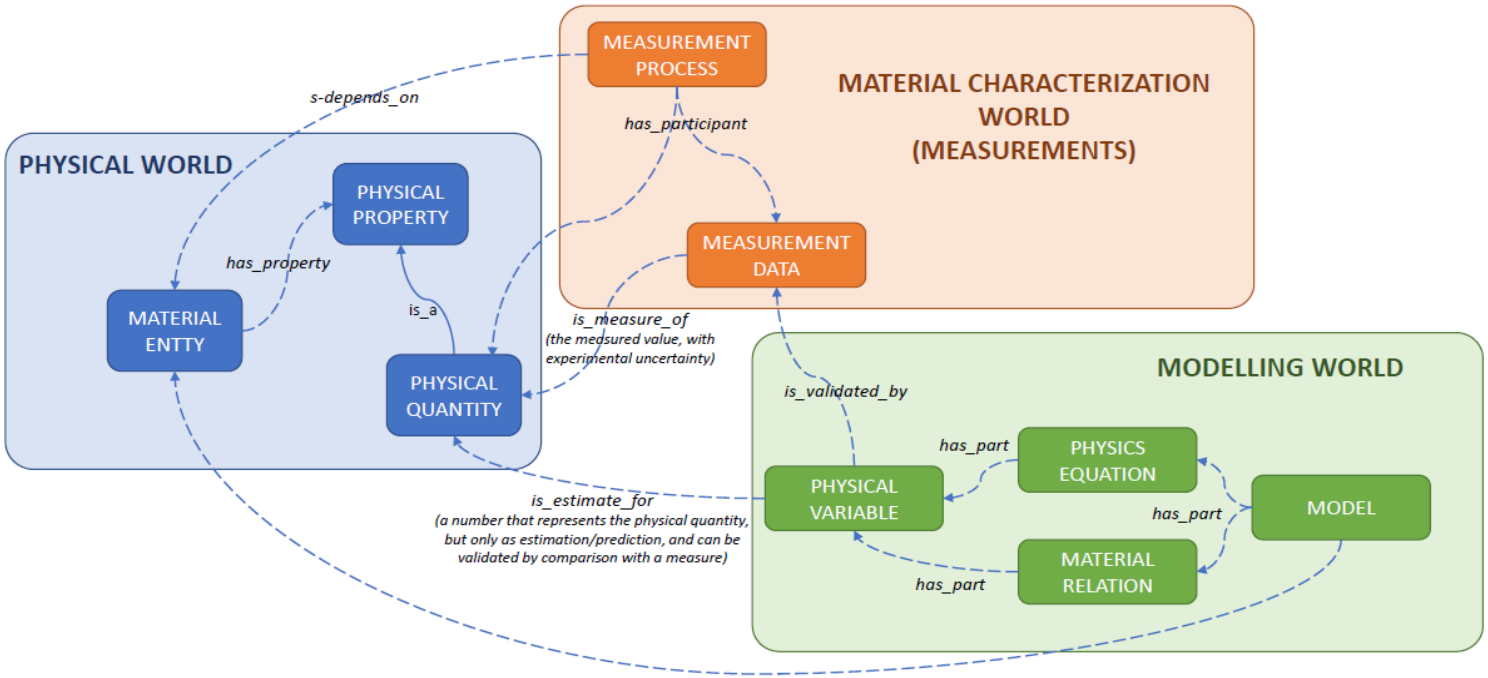
BattINFO: the Battery Interface Ontology

- Creating the language to connect the different battery worlds
- Read more about the BattINFO ontology at the website or watch the video



Simon Clark, Jesper Friis and others (SINTEF)

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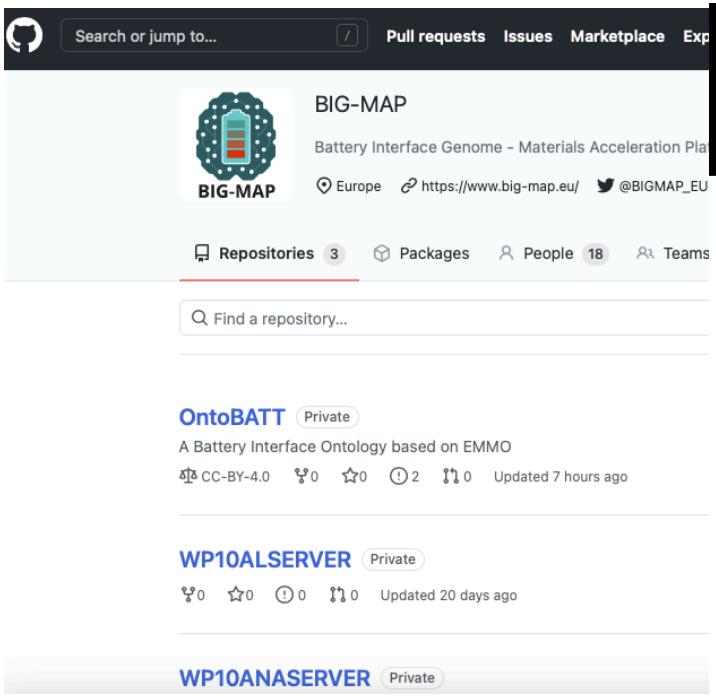
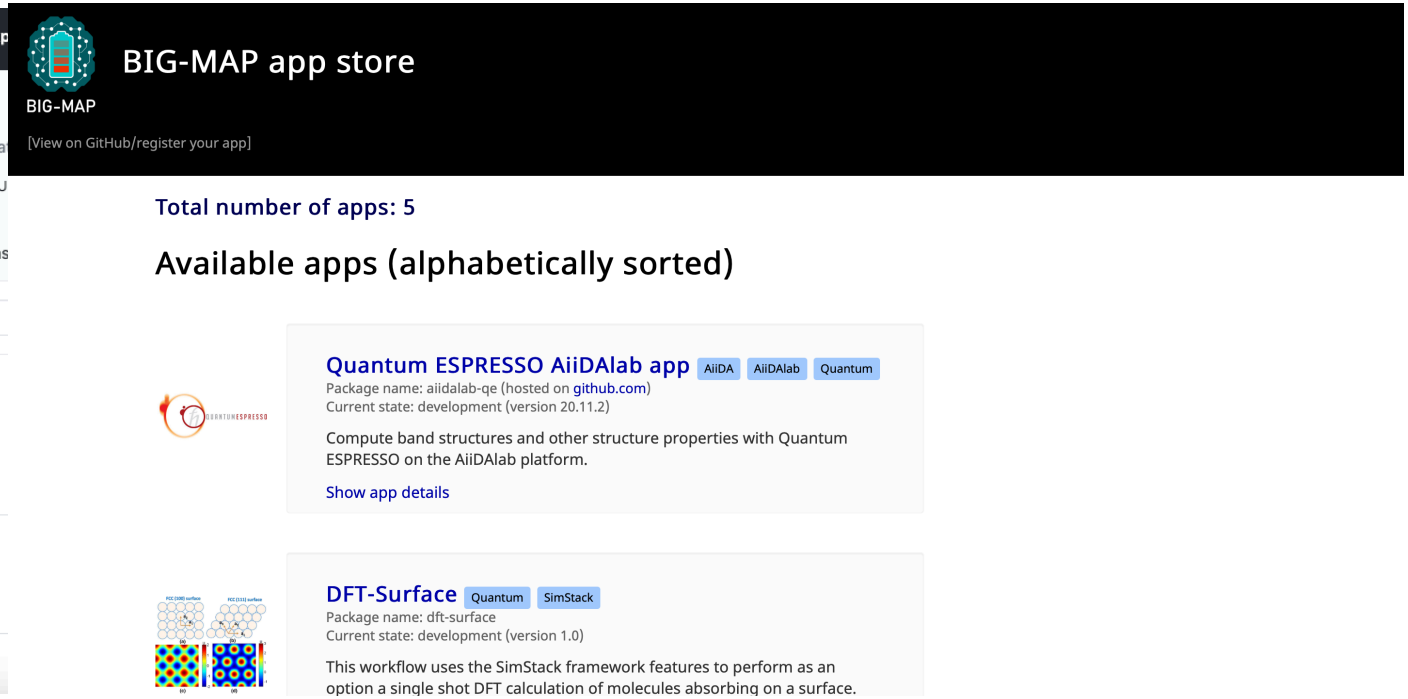
BIG-MAP App Store and registry (GitHub)

- Developing externalizable tools for the European battery community
- We've created a BIG-MAP registry (GitHub) and a BIG-MAP App Store
- …more about this after the three presentations





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