Smart Functionalities: Manufacturability and Accelerated Materials Discovery

Project update from BatCAT

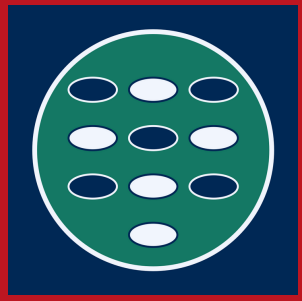
Battery2030+ Annual Conference
Münster, 6th May 2025

Fakultet for realfag og teknologi

Forskargruppe materialteori og -informatikk

Noregs miljø- og biovitskaplege universitet

Materialteori og -informatikk



Digitalisering på Ås

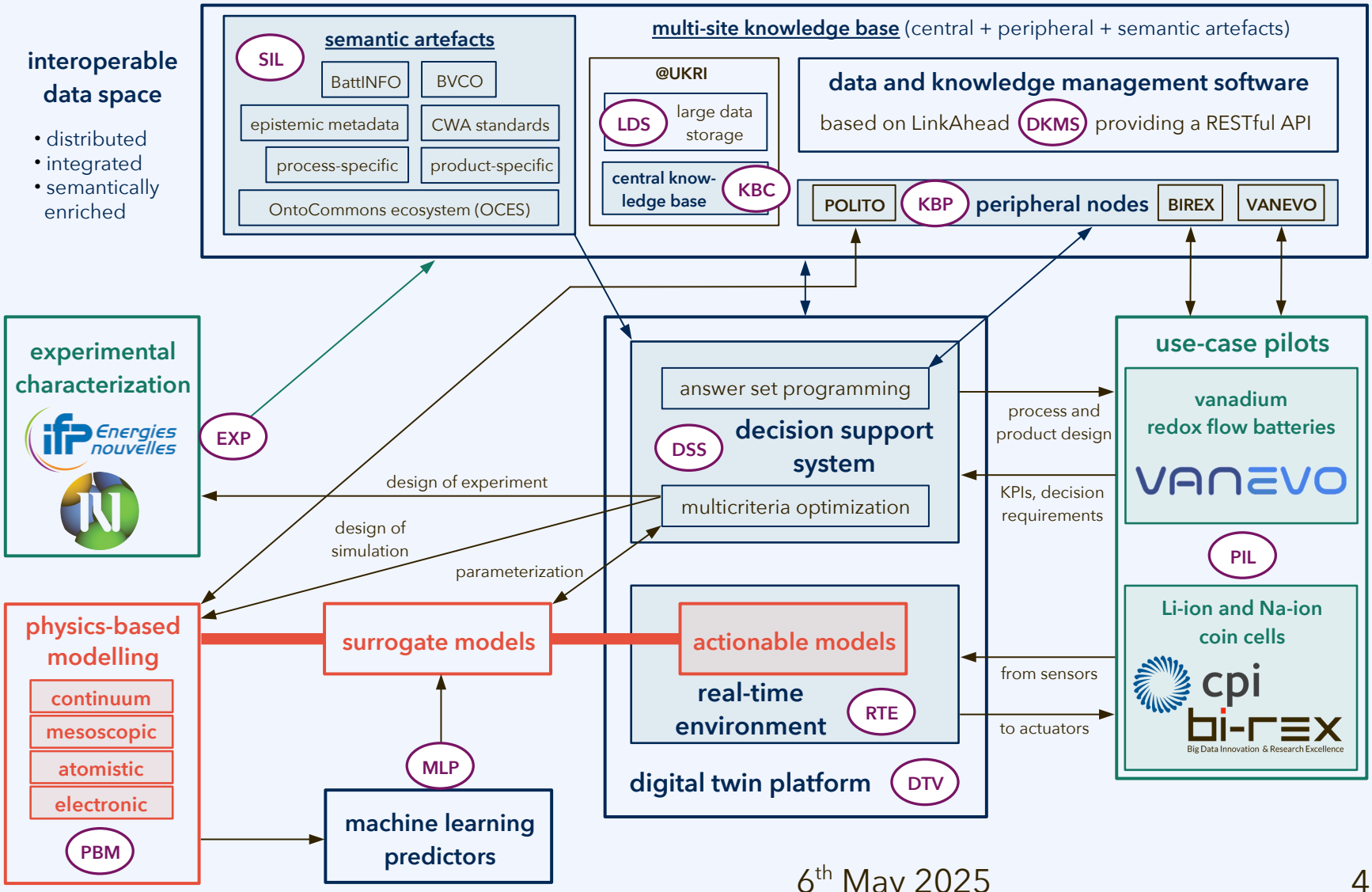
BatCAT Battery Cell Assembly Twin

1. **Project overview and status**
2. *Simulation campaign plan*
3. *Core and mid ontologies*

BatCAT project summary

- BatCAT is one of the two projects, alongside BATTwin, that realize the BATTERY 2030+ manufacturability programme from 2024 to 2027 by developing a **digital twin platform** and **data space** for battery manufacturing.
- BatCAT primarily considers **vanadium redox-flow batteries** (**VANEVO pilot**) as well as Li-ion & Na-ion coin cells (CPI pilot + associated pilot at IfE).
- **MCO** and **logic programming** will be used for a decision support system.
- Simulation methods cover all from quantum mechanical DFT over **molecular simulation** with classical pair potentials, mesoscopic methods such as DPD with nDPD potentials, and **continuum models**, *e.g.*, based on the Poisson-Nernst-Planck equation, as well as population balance models.
- **Time-series predictors** will include cellular neural networks with potential for embedded system deployment.

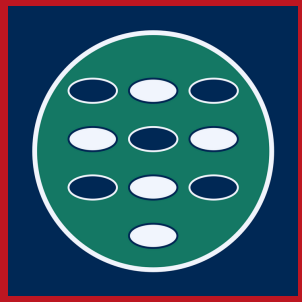
BatCAT project summary



Status update M15 (March 2025)

- Core ontology and mapping to answer set programming drafted (MS8).
  - **Core ontology** drafting: Internal work, so far
  - **Mid-level ontologies** (MSO-EM): https://github.com/HE-BatCAT/mso-em
- Delivery of the risk management plan (D8.3).
- Documentation: All pilot line & sensorics equipment will be in place (MS9).
- Update of the communication, dissemination, and training plan (MS10).
- For five key tasks: Controlled that they are in line with requirements (MS7).

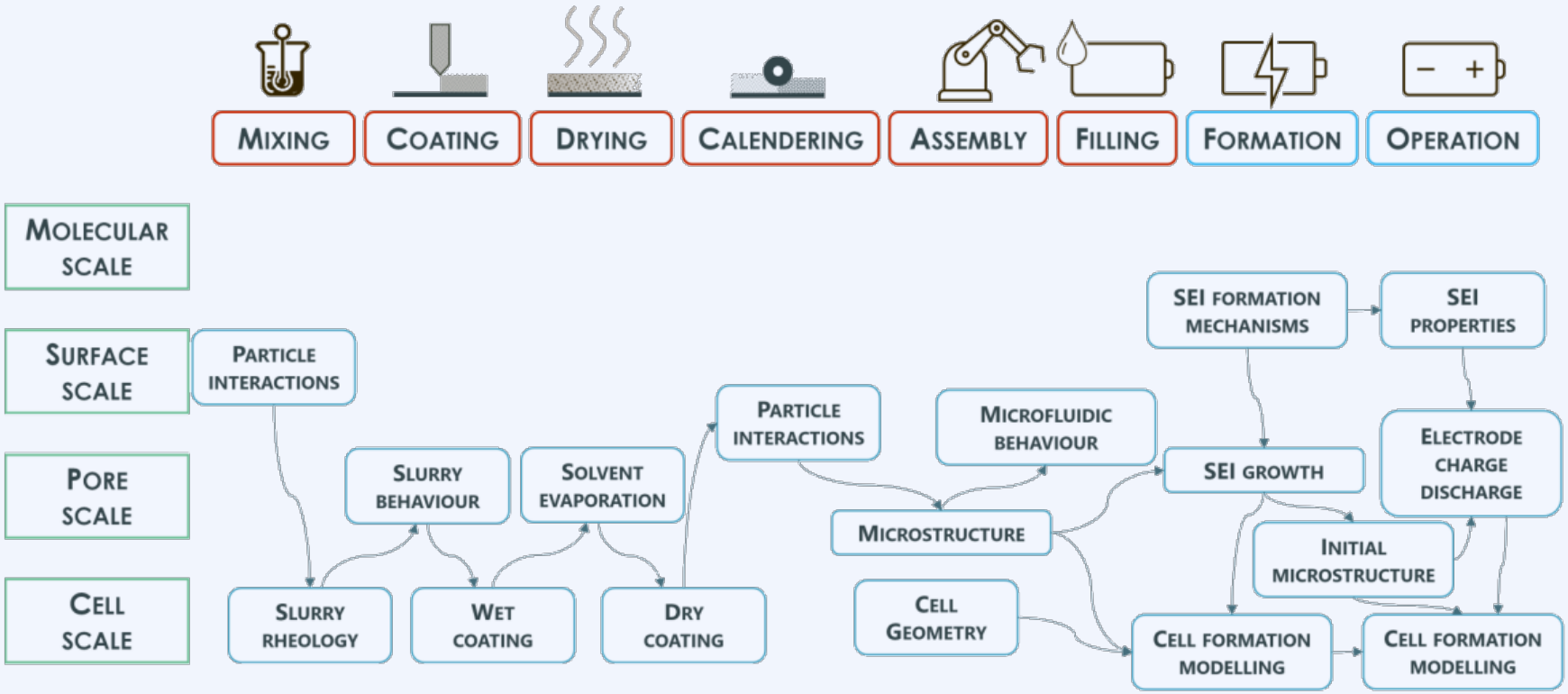
Noregs miljø- og biovitskaplege universitet



BatCAT
Battery Cell Assembly Twin

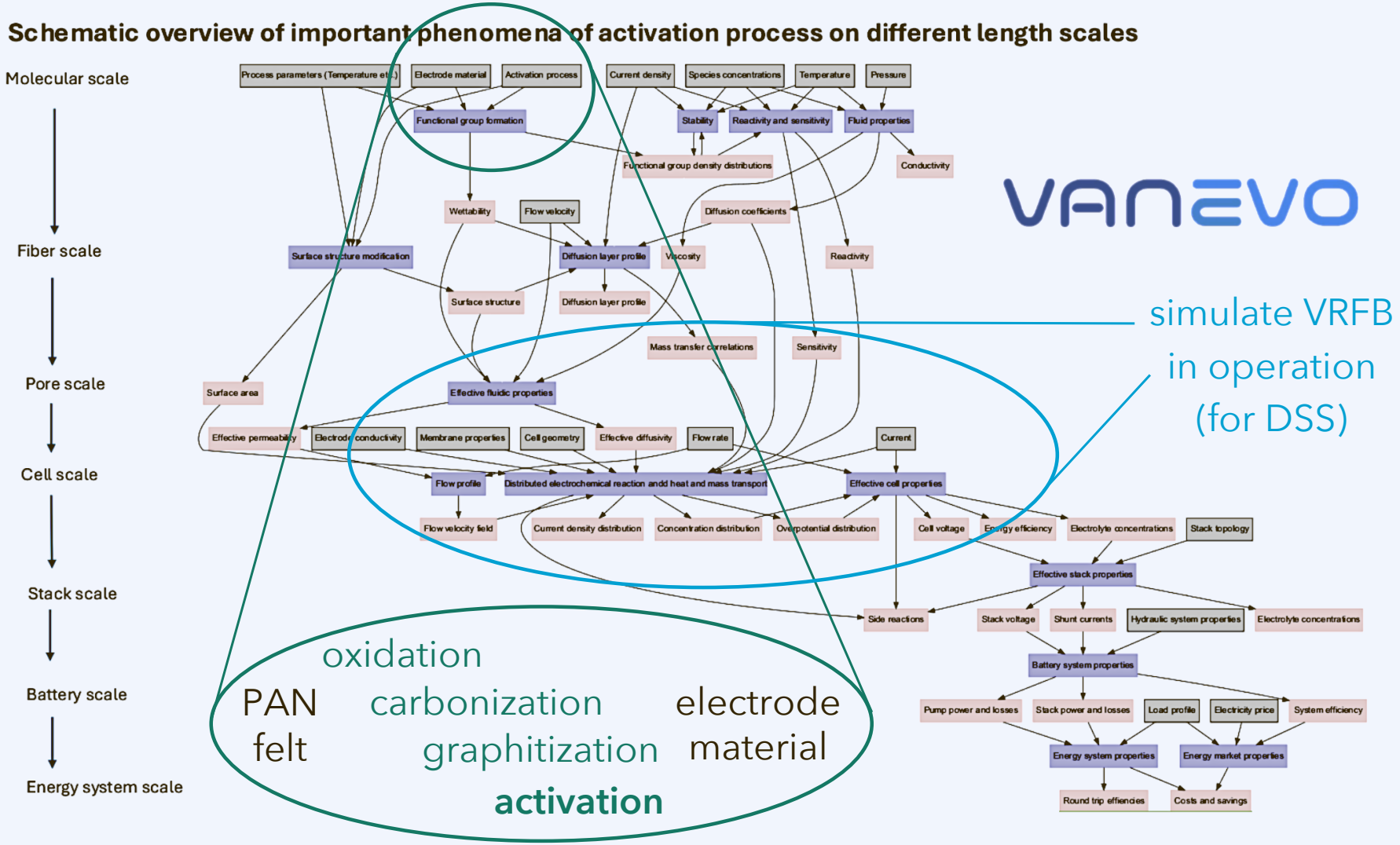
1. Project overview and status
2. **Simulation campaign plan**
3. *Core and mid ontologies*

Li-ion & Na-ion simulation requirements

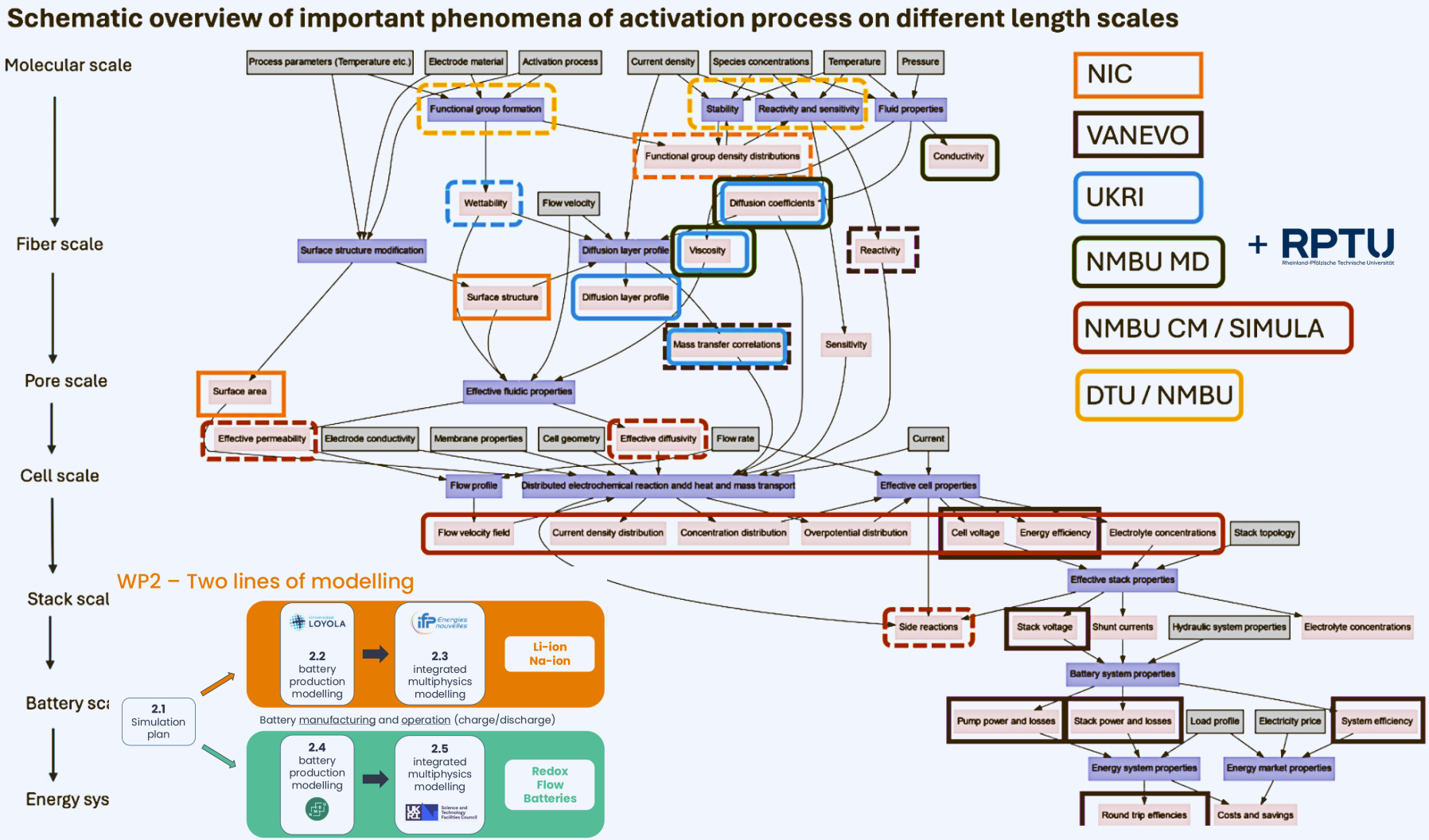


Li-ion and Na-ion use case schematic. (Used for the simulation campaign plan.)

VRFB simulation requirements



Multiphysics simulation in BatCAT



Multiphysics simulation in BatCAT

For the redox-flow use case:

For both use cases:

MicTherm
coupling/
linking

RPTU
Rheinland-Pfälzische Technische Universität

MolMod DB
model
repository

RPTU
Rheinland-Pfälzische Technische Universität

proprietary
MCO tool

Fraunhofer ITWM

We are also exploring free MCO tools.

Modelling VRFB operation (for DSS):

MD using ms2

RPTU
Rheinland-Pfälzische Technische Universität

surrogate

surrogate

surrogate

UKRI Science and Technology Facilities Council

DPD using DL_MESO

continuum models
using FEniCS

simula

surrogate

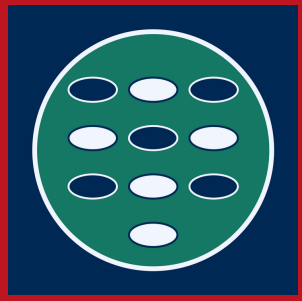
MCO, **ASP**, and **actionable modelling**

Modelling electrode
activation: DFT (QM)

DTU

Noregs miljø- og biovitskaplege universitet

Materialteori og -informatikk

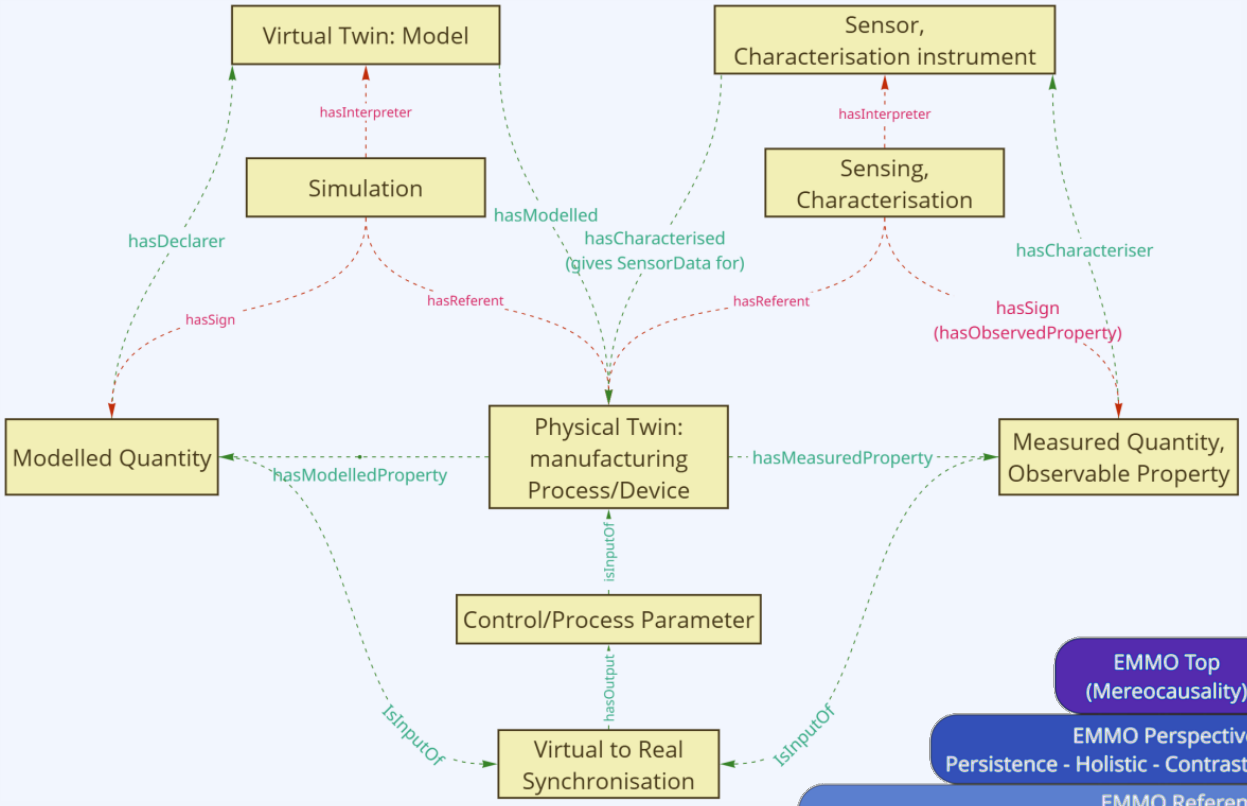


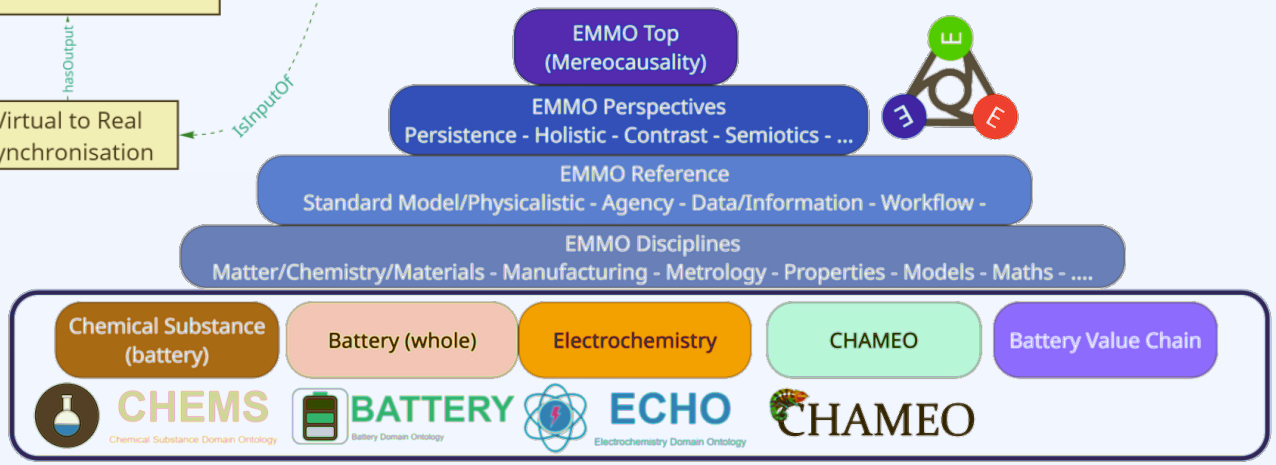
Digitalisering på Ås

BatCAT Battery Cell Assembly Twin

1. Project overview and status
2. Simulation campaign plan
3. **Core and mid ontologies**

BatCAT core ontology: Early drafting





Mid-level ontology development

European AI Act: "To address concerns related to **opacity** and […] fulfil their obligations under this Regulation, **transparency** should be required for high-risk AI systems before they are placed on the market […]. High-risk AI systems should […] enable deployers to understand how the AI system works […]. High-risk AI systems should be accompanied by **appropriate information**".

Epistemic opacity can occur when simulation-based and data-driven methods are used. The concept was introduced by **Humphreys** in *Extending Ourselves*[1] (2004), developed further in later work,[2] and has had a substantial impact.[3]

> **Epistemic opacity** (Humphreys, 2011): A «process is **epistemically opaque** relative to a cognitive agent *X* at time *t* […if …] *X* does not know at *t* all of the **epistemically relevant elements**»[2]

[1]P. Humphreys, *Extending Ourselves Computational Science, Empiricism, and Scientific Method*, **2004**.

[2]P. Humphreys, in M. Carrier, A. Nordmann, *Science in the Context of Application*, *pp.* 131–142, Springer, **2011**.

[3]J. M. Durán, N. Formanek, *Minds and Machines* **28**(4): 645–666, doi:10.1007/s11023-018-9481-6, **2018**.

Mid-level ontology development

Epistemic metadata are the information that **establishes the knowledge status** of data or digital objects.[1, 2]

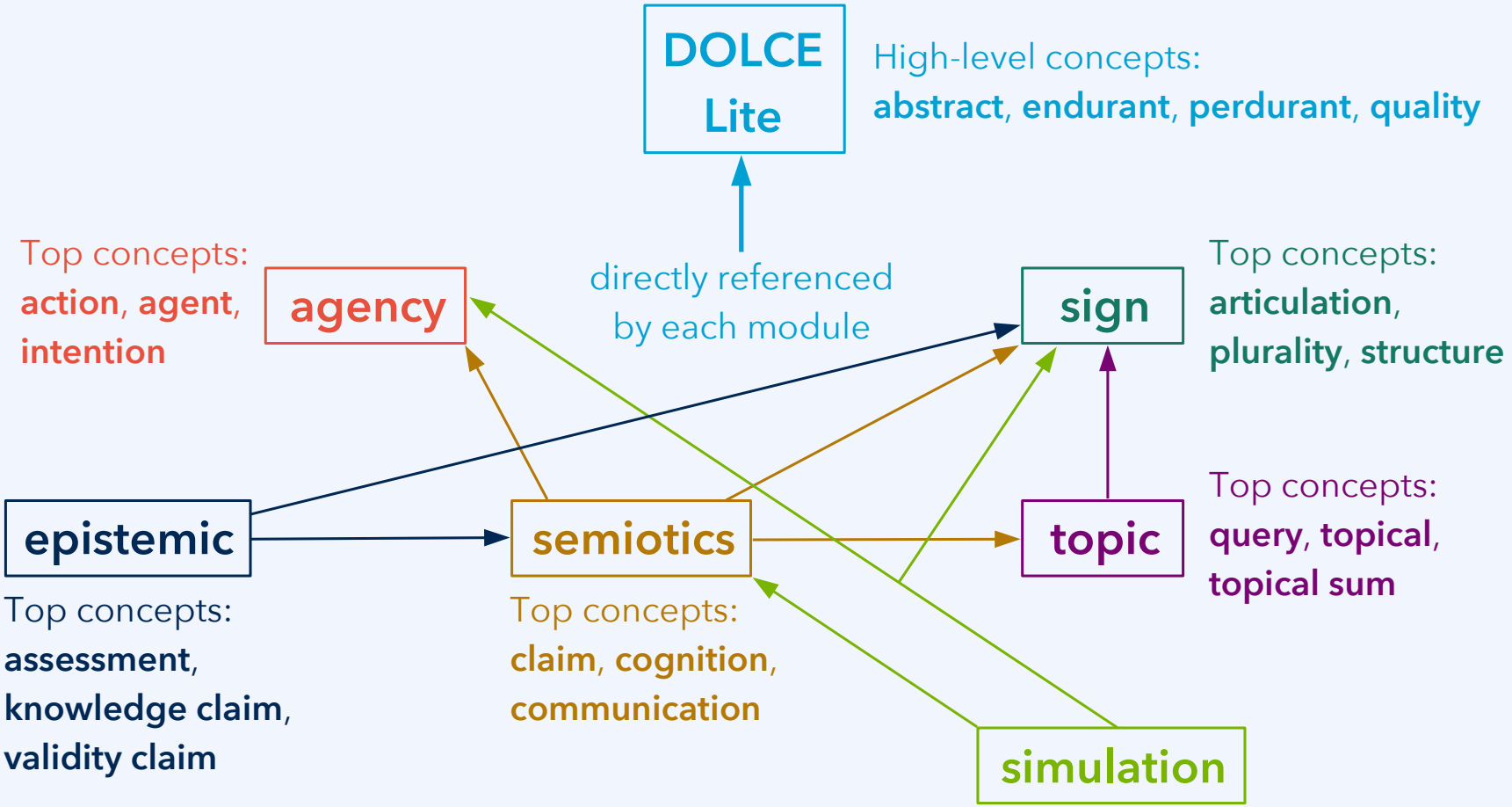
Questions we must answer to establish the knowledge status:

a) "what **knowledge claim φ** has been formulated?,"
b) "where do the data and the claim come from?" (**provenance**),
c) "what **validity claim** was made about φ?,"
d) "why should we accept any of this?" (**grounding**).

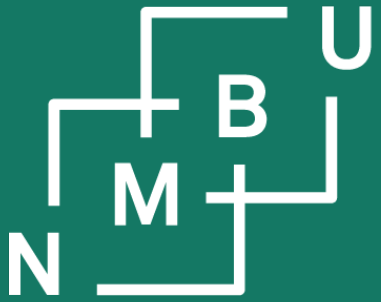
Key epistemic metadata items are the **knowledge claims** made based on data, their **provenance**, **validation** and **reproducibility**, and **epistemic grounding**.

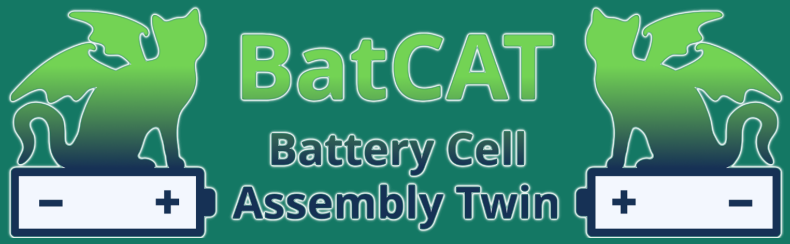
[1] In *Proc. JOWO 2022*, CEUR *vol.* **3249**: *p. 2 (CAOS)*, CEUR-WS, **2022**.
[2] In *Proc. FOIS 2023*, *pp.* 302–319, doi:10.3233/faia231136, IOS, **2023**.

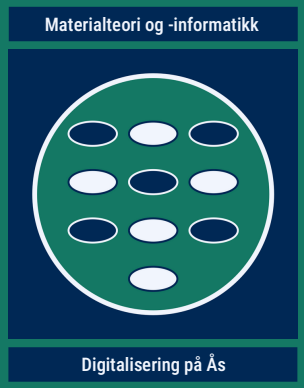
Mid-level ontology development



Remaining four additional modules:
explanation, **observation**, **quantity**, **reliability**.







BatCAT has received funding from the European Union's **Horizon Europe** research and innovation programme under **grant agreement no. 101137725**. Views and opinions expressed are however those of the authors only and do not necessarily reflect those of the project, the European Climate, Infrastructure and Environment Executive Agency (CINEA), or the European Union. Neither BatCAT nor the CINEA or the EU can be held responsible for them.

Finansiert av Den europeiske union

6st May 2025

NMBU Fakultet for realfag og teknologi Forskargruppe materialteori og -informatikk

Smart Functionalities: Manufacturability and Accelerated Materials Discovery

Project update from BatCAT

Battery2030+ Annual Conference
Münster, 6th May 2025

Fakultet for realfag og teknologi

Forskargruppe materialteori og -informatikk